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L5               TRANSFER  PLU=ON  L4 1- RN :   22168 TERMS
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                  OR NI OR CO)/ELS
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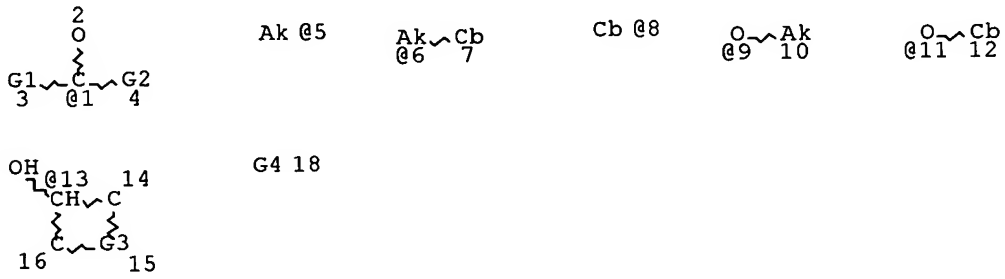


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L19  ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:908108  CAPLUS  Full-text
DOCUMENT NUMBER:          147:406255
TITLE:                    C-H bond activation by water on a palladium or
                          platinum metal surface
AUTHOR(S):                Matsubara, Seijiro; Asano, Keisuke; Kajita, Yuichi;
                          Yamamoto, Mitsuru
CORPORATE SOURCE:         Department of Material Chemistry, Graduate School of
                          Engineering, Kyoto University, Kyoudai-katsura, Kyoto,
                          606-8501, Japan
SOURCE:                   Synthesis (2007), (13), 2055-2059
                          CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER:                Georg Thieme Verlag
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 147:406255
AB    A water mol. is partially cleaved on a palladium or platinum metal surface
      under hydrothermal conditions to form an active platinum species.  The species
      is effective for C-H bond functionalization which can be applied for H/D-
      exchange reactions, C-C bond-forming reactions, and C-N bond-forming
      reactions.
CC    22-4 (Physical Organic Chemistry)
      Section cross-reference(s): 66, 67
IT    Deuteration
        Deuteration catalysts
          (C-H bond activation by water on a palladium or platinum metal surface)
IT    1314-08-5, Palladium oxide (PdO) 1314-15-4, Platinum
      oxide (PtO2) 3375-31-3 7440-05-3, Palladium, uses
      7440-06-4, Platinum, uses  7440-44-0, Carbon, uses
      7718-54-9, Nickel chloride, uses
      RL: CAT (Catalyst use); USES (Uses)
          (C-H bond activation by water on a palladium or platinum metal surface)
IT    111-67-1P, 2-Octene  112-40-3P, Dodecane  592-98-3P, 3-Octene
      592-99-4P, 4-Octene  10249-89-5P  20617-93-0P, Quinoxaline-2,3,5,6,7,8-
      d6  25378-22-7P, Dodecene  32190-42-4P  34071-94-8P, Quinoline-d7
      36340-20-2P  73509-20-3P, 1H-Indole-1,2,3,4,5,6,7-d7  97797-70-1P
      97960-58-2P  132125-39-4P  634897-78-2P  688320-42-5P  688320-43-6P
      688320-44-7P  688320-45-8P  688320-46-9P 688320-48-1P
```

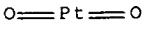
880462-22-6P 951164-39-9P 951164-40-2P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(C-H bond activation by water on a palladium or platinum metal surface)

IT **7440-02-0**, Raney nickel, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts; C-H bond activation by water on a palladium or platinum metal surface)

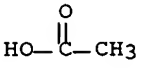
IT **1314-08-5**, Palladium oxide (PdO) **1314-15-4**, Platinum oxide (PtO2) **3375-31-3 7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses **7718-54-9**, Nickel chloride, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(C-H bond activation by water on a palladium or platinum metal surface)

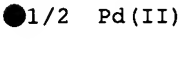
RN 1314-08-5 CAPLUS
CN Palladium oxide (PdO) (CA INDEX NAME)

RN 1314-15-4 CAPLUS
CN Platinum oxide (PtO2) (CA INDEX NAME)



RN 3375-31-3 CAPLUS
CN Acetic acid, palladium(2+) salt (2:1) (CA INDEX NAME)

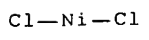




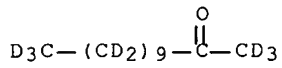
RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

RN 7718-54-9 CAPLUS
CN Nickel chloride (NiCl2) (CA INDEX NAME)



IT **688320-48-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(C-H bond activation by water on a palladium or platinum metal surface)
RN 688320-48-1 CAPLUS
CN 2-Dodecanone-1,1,1,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-d24 (CA INDEX NAME)



IT **7440-02-0**, Raney nickel, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts; C-H bond activation by water on a palladium or platinum metal surface)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:609303 CAPLUS Full-text
DOCUMENT NUMBER: 147:52633
TITLE: Process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems
INVENTOR(S): Heller, Detleff; Buschmann, Helmut; Drexler, Hans-Joachim
PATENT ASSIGNEE(S): Laboratorios Del Dr. Esteve, S.A., Spain
SOURCE: Eur. Pat. Appl., 11pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 1792887	A1	20070606	EP 2005-384038 20051205
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU			
WO 2007065891	A1	20070614	WO 2006-EP69313 20061205
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: EP 2005-384038 A 20051205
OTHER SOURCE(S): CASREACT 147:52633; MARPAT 147:52633

AB A process for the catalytic hydrogenation/deuteration of C1-6 alkyl ketones, e.g., acetone, (including prochiral ketones) or their deuterated derivs. in high yield and selectivity into their resp. secondary alkanols, e.g., isopropanol, is described. This process comprises using ruthenium achiral or chiral catalytic systems to yield racemic or nonracemic chiral alcs. or deuterated racemic or nonracemic chiral alcs. under high pressure and room temperature

CC 23-8 (Aliphatic Compounds)
Section cross-reference(s): 67

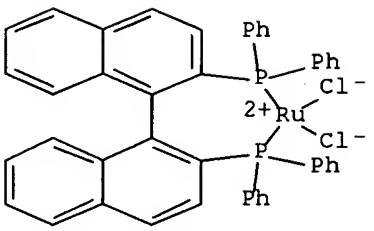
IT **Deuteration**
Deuteration catalysts
Hydrogenation
Hydrogenation catalysts
(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

IT 29841-69-8 **134524-84-8 925941-06-6 939824-57-4 939824-58-5**
RL: **CAT (Catalyst use)**; USES (Uses)
(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

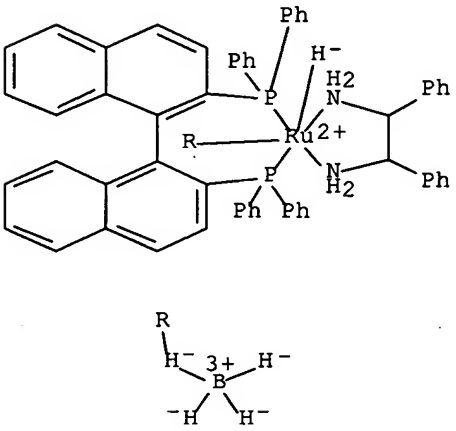
IT **3976-29-2P**, 2-Propan-1,1,1,3,3,3-d6-ol
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

IT **134524-84-8 925941-06-6 939824-57-4 939824-58-5**
RL: **CAT (Catalyst use)**; USES (Uses)
(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)

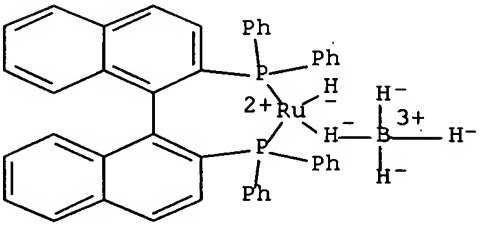
RN 134524-84-8 CAPLUS
CN Ruthenium, [(1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenylphosphine-κP]]dichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 925941-06-6 CAPLUS
CN Ruthenium, [1,1'-(1S)-[1,1'-binaphthalene]-2,2'-diylbis[1,1-diphenylphosphine-κP]][(1S,2S)-1,2-diphenyl-1,2-ethanediamine-κN1,κN2]hydro[tetrahydroborato(1-)-κH]-, (OC-6-22)- (CA INDEX NAME)



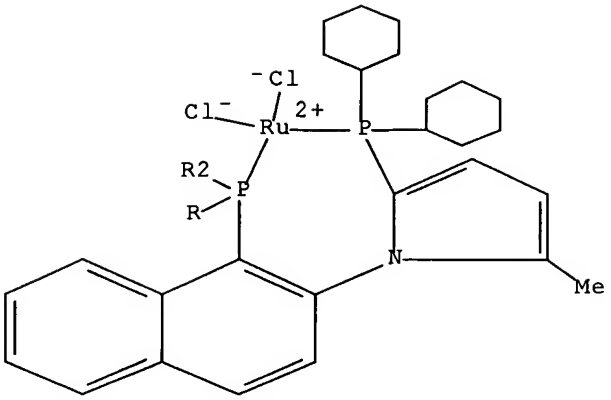
RN 939824-57-4 CAPLUS
CN Ruthenium, [1,1'-[1,1'-binaphthalene]-2,2'-diylbis[1,1-diphenylphosphine-κP]]hydro[tetrahydroborato(1-)-κH]- (CA INDEX NAME)



RN 939824-58-5 CAPLUS
CN Ruthenium, dichloro[2-(dicyclohexylphosphino-κP)-1-[1-(dicyclohexylphosphino-κP)-2-naphthalenyl]-5-methyl-1H-pyrrole]-

(CA INDEX NAME)

PAGE 1-A



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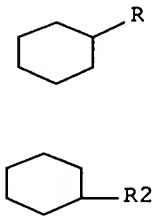
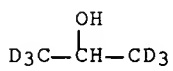


IT **3976-29-2P**, 2-Propan-1,1,1,3,3,3-d6-ol
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(process for the homogeneous hydrogenation/deuteration of ketones into their corresponding secondary alkanols using ruthenium catalytic systems)
RN 3976-29-2 CAPLUS
CN 2-Propan-1,1,1,3,3,3-d6-ol (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1014792 CAPLUS Full-text
DOCUMENT NUMBER: 146:7638
TITLE: C-H/C-D exchange reactions of aromatic compounds in

D2O with NaBD4-activated catalysts
AUTHOR(S): Derdau, Volker; Atzrodt, Jens
CORPORATE SOURCE: GMPK, Isotope Chemistry & Metabolite Synthesis Frankfurt, Sanofi-Aventis Deutschland GmbH, Frankfurt/Hoechst, 65926, Germany
SOURCE: Synlett (2006), (12), 1918-1922
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:7638

AB A safe and efficient method for catalytic H/D exchange to provide high deuterium incorporation into a variety of aromatic substrates was developed. Systematic screening of the catalyst and activator revealed that the essential activation of the Pd catalyst could be achieved under safe and user friendly conditions. The application of this simple catalytic method for the deuteration of bi- and tricyclic aromatic compds. and chiral natural products was investigated.

CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 27

IT **Deuteration**
Deuteration catalysts
(C-H/C-D exchange reactions of aromatic compds. in D2O with NaBD4-activated catalysts)

IT **7440-05-3**, Palladium, uses **7647-10-1**, Palladium(II) chloride
RL: **CAT (Catalyst use)**; USES (Uses)
(C-H/C-D exchange reactions of aromatic compds. in D2O with NaBD4-activated catalysts)

IT **37464-79-2P** 651316-73-3P 915232-04-1P 915232-06-3P 915232-14-3P 915232-16-5P 915232-18-7P 915232-20-1P 915232-22-3P 915232-24-5P 915232-26-7P 915232-28-9P 915232-30-3P 915232-33-6P 915232-35-8P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(C-H/C-D exchange reactions of aromatic compds. in D2O with NaBD4-activated catalysts)

IT **7440-05-3**, Palladium, uses **7647-10-1**, Palladium(II) chloride
RL: **CAT (Catalyst use)**; USES (Uses)
(C-H/C-D exchange reactions of aromatic compds. in D2O with NaBD4-activated catalysts)

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

RN 7647-10-1 CAPLUS
CN Palladium chloride (PdCl2) (CA INDEX NAME)

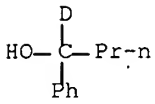
Cl—Pd—Cl

IT **37464-79-2P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**
(C-H/C-D exchange reactions of aromatic compds. in D2O with NaBD4-activated catalysts)

RN 37464-79-2 CAPLUS

CN Benzenemethan-d-ol, α-propyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:689620 CAPLUS Full-text
DOCUMENT NUMBER: 146:421688
TITLE: Synergistic effect of a palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reactions of alkyl-substituted aromatic compounds
AUTHOR(S): Ito, Nobuhiro; Watahiki, Tsutomu; Maesawa, Tsuneaki; Maegawa, Tomohiro; Sajiki, Hironao
CORPORATE SOURCE: Chemical Products Research Laboratories, Wako Pure Chemical Industries, Ltd., 1633 Matoba, Kawagoe, 350-1101, Japan
SOURCE: Advanced Synthesis & Catalysis (2006), 348(9), 1025-1028
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A synergistic effect in the H-D exchange reaction of alkyl-substituted aromatic compds. using the Pd/C-Pt/C-D2O-H2 system was discovered. This system would lead to fully H-D exchange results even on the sterically hindered sites which were only low-deuterium incorporated by Pd/C or Pt/C independently. Since the reaction was general for a variety of aromatic compds., it could be applied to the deuteration of dianiline derivs. as raw materials for polyimides.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Deuteration**
Deuteration catalysts
Exchange reaction
Exchange reaction catalysts
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

IT **7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

IT **767627-97-4P**, Benzene-d5-pentanoic-d8 acid 861405-62-1P
870284-54-1P 870284-60-9P 870284-63-2P 870284-66-5P 870284-69-8P
934266-51-0P 934266-52-1P **934266-54-3P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

IT **7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

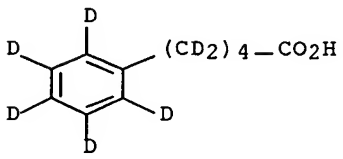
Pd

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

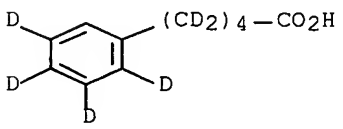
Pt

IT **767627-97-4P**, Benzene-d5-pentanoic-d8 acid **934266-54-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)

RN 767627-97-4 CAPLUS
CN Benzene-d5-pentanoic-d8 acid (CA INDEX NAME)



RN 934266-54-3 CAPLUS
CN Benzene-2,3,4,5-d4-pentanoic-α,α,β,β,γ,γ,δ,δ-d8 acid (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:108991 CAPLUS Full-text
DOCUMENT NUMBER: 144:292970
TITLE: Synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide
AUTHOR(S): Esaki, Hiroyoshi; Aoki, Fumiyo; Maegawa, Tomohiro; Hirota, Kosaku; Sajiki, Hironao
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Gifu Pharmaceutical University, Mitahora-higashi, Gifu, 502-8585, Japan
SOURCE: Heterocycles (2005), 66, 361-369
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:292970

AB The D2 gas-free and base-selective H-D exchange reaction of nucleosides was developed. It discloses a convenient route to the post-synthetic incorporation of deuteriums into the base moiety of nucleic acids with high deuterium efficiency.

CC 33-9 (Carbohydrates)

IT **Deuteration**
(regioselective; synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT **Deuteration catalysts**
(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT 24897-52-7P, 2,4(1H,3H)-Pyrimidinedione-5,6-d2 **28671-50-3P**, Cytidine-5-d **40436-51-9P**, Uridine-5-d **40632-21-1P**, Uridine-5,6-d2 **40632-25-5P**, Cytidine-5,6-d2 **74848-84-3P**, Thymidine-α,α,α-d3 **82845-88-3P**, Adenosine-2,8-d2 90742-80-6P **96412-41-8P**, Guanosine-8-d 102147-86-4P 106391-24-6P 200496-79-3P 697807-00-4P, 1H-Purin-2,8-d2-6-amine **697807-01-5P**, Inosine-2,8-d2 697807-02-6P **860788-48-3P** **879005-77-3P**, Thymidine-α-d **879005-78-4P**, Thymidine-α,α-d2
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

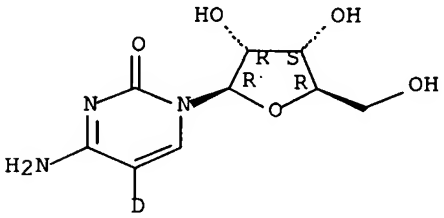
RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

IT **28671-50-3P**, Cytidine-5-d **40436-51-9P**, Uridine-5-d
40632-21-1P, Uridine-5,6-d2 **40632-25-5P**, Cytidine-5,6-d2
74848-84-3P, Thymidine-α,α,α-d3
82845-88-3P, Adenosine-2,8-d2 **96412-41-8P**, Guanosine-8-d
697807-01-5P, Inosine-2,8-d2 **860788-48-3P**
879005-77-3P, Thymidine-α-d **879005-78-4P**,
Thymidine-α,α-d2
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(synthesis of base-selectively deuterium-labeled nucleosides by the pd/C-catalyzed H-D exchange reaction in deuterium oxide)

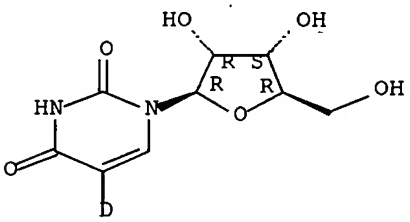
RN 28671-50-3 CAPLUS
CN Cytidine-5-d (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



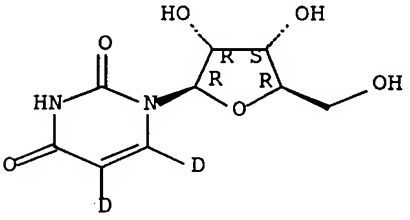
RN 40436-51-9 CAPLUS
CN Uridine-5-d (9CI) (CA INDEX NAME)

Absolute stereochemistry.



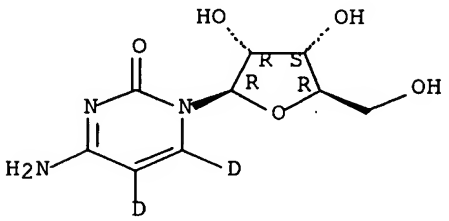
RN 40632-21-1 CAPLUS
CN Uridine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



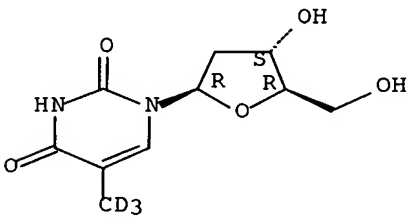
RN 40632-25-5 CAPLUS
CN Cytidine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



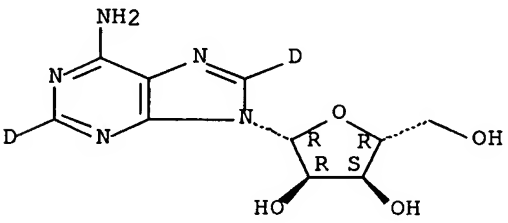
RN 74848-84-3 CAPLUS
CN Thymidine-α,α,α-d3 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



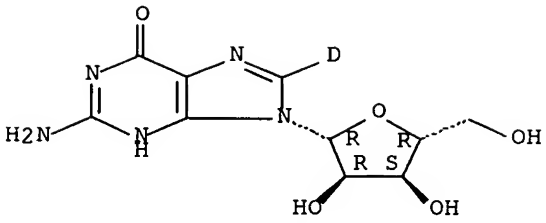
RN 82845-88-3 CAPLUS
CN Adenosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



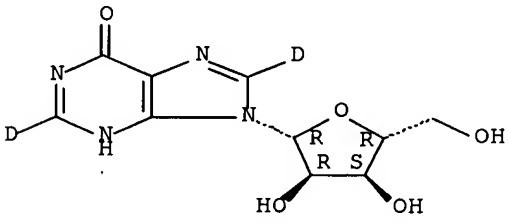
RN 96412-41-8 CAPLUS
CN Guanosine-8-d (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



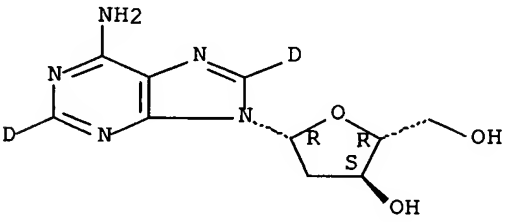
RN 697807-01-5 CAPLUS
CN Inosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



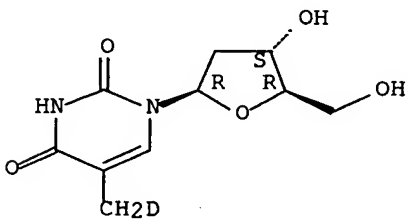
RN 860788-48-3 CAPLUS
CN Adenosine-2,8-d2, 2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



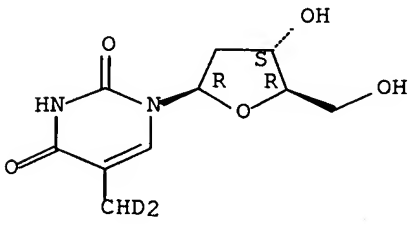
RN 879005-77-3 CAPLUS
CN Thymidine-α-d (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 879005-78-4 CAPLUS
CN Thymidine-α,α-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:696848 CAPLUS Full-text
DOCUMENT NUMBER: 143:172769
TITLE: Method of deuteration of aromatic ring and/or heterocycle compounds using mixed metal catalyst
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070853	A1	20050804	WO 2004-JP19049	20041221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2553376	A1	20050804	CA 2004-2553376	20041221
EP 1707548	A1	20061004	EP 2004-807406	20041221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1906143	A	20070131	CN 2004-80040874	20041221
PRIORITY APPLN. INFO.:			JP 2004-16075 A	20040123
			WO 2004-JP19049 W	20041221

AB A method of deuteration in which a compound with aromatic ring and/or heterocycle having an enhanced deuteration ratio can be obtained. There is provided a method of deuterating a compound with aromatic ring and/or

heterocycle, characterized in that a compound with aromatic ring and/or heterocycle is reacted with a deuterium source in the presence of an activated mixed catalyst composed of at least two members selected from among a palladium catalyst, a platinum catalyst, a rhodium catalyst, an iridium catalyst, a ruthenium catalyst, a nickel catalyst and a cobalt catalyst. Thus, 500 mg nicotinic acid, 50 mg Pd/C (5 mg Pd), and 100 mg Pt/C (5 mg Pt) were suspended in 17 mL D2O, sealed, purged with H, and heated at 180° for .apprx.24 h to give deuterated nicotinic acid with 99% deuteration at 2, 5, and 6 positions and 48% deuteration at 4 position vs. 98% deuteration at 2 and 5 positions, 99% deuteration at 6 position, and 10% deuteration at 4 position when Pd/C was used alone.

IC ICM C07B059-00
ICS C07C037-00; C07C039-06; C07C051-00; C07C057-30; C07C063-04; C07C211-45; C07C209-00; C07D213-803; C07D213-74; C07B061-00; C07M005-00

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25

IT **Deuteration**
Deuteration catalysts
(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT **Deuteration**
Deuteration catalysts
(regioselective; method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT 7439-88-5, Iridium, uses **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-18-8**, Ruthenium, uses **7440-48-4**, Cobalt, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT 1821-12-1P, 4-Phenylbutanoic acid 2438-05-3DP, deuterated derivative 7128-85-0P 7217-47-2DP, deuterated derivative 22527-01-1DP, deuterated derivative 22527-01-1P 66148-15-0P 87385-38-4DP, deuterated derivative **134860-14-3DP**, Benzenebutanoic-α,α,β,β,.gamma.a.,γ-d6 acid, deuterated derivative **358730-86-6P**, Benzene-d5-butanoic-d6 acid **767627-97-4P**, Benzene-d5-pentanoic-d8 acid **861405-57-4DP**, Benzenepentanoic-d8 acid, deuterated derivative **861405-58-5DP**, Benzene-3,4,5-d3-pentanoic acid, deuterated derivative **861405-59-6DP**, deuterated derivative **861405-60-9DP**, Benzene-3,4,5-d3-butanoic acid, deuterated derivative 861405-61-0DP, deuterated derivative 861405-62-1P 861405-63-2P 861405-64-3DP, deuterated derivative 861405-65-4P 861405-66-5DP, deuterated derivative 861405-67-6DP, deuterated derivative 861405-68-7P 861405-69-8P 861405-70-1DP, deuterated derivative 861405-71-2P 861405-72-3P 861405-73-4DP, deuterated derivative 861405-74-5DP, deuterated derivative 861405-75-6P 861405-76-7DP, 3-Pyridine-6-d-carboxylic acid, deuterated derivative
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

IT **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-18-8**, Ruthenium, uses **7440-48-4**, Cobalt, uses

RL: **CAT (Catalyst use)**; USES (Uses)
(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

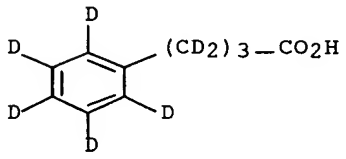
RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

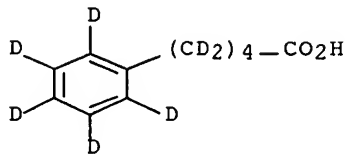
IT **134860-14-3DP**, Benzenebutanoic-α,α,β,β,.gamm
a.,γ-d6 acid, deuterated derivative **358730-86-6P**,
Benzene-d5-butanoic-d6 acid **767627-97-4P**, Benzene-d5-pentanoic-
d8 acid **861405-57-4DP**, Benzenepentanoic-d8 acid, deuterated
derivative **861405-58-5DP**, Benzene-3,4,5-d3-pentanoic acid,
deuterated derivative **861405-59-6DP**, deuterated derivative
861405-60-9DP, Benzene-3,4,5-d3-butanoic acid, deuterated derivative
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(method of deuteration of aromatic ring and/or heterocycle compds. using
mixed metal catalyst such as palladium and platinum on carbon)
RN 134860-14-3 CAPLUS
CN Benzenebutanoic-α,α,β,β,γ,γ-d6 acid
(9CI) (CA INDEX NAME)

Ph—$(CD_2)_3$—CO_2H

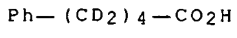
RN 358730-86-6 CAPLUS
CN Benzene-d5-butanoic-d6 acid (9CI) (CA INDEX NAME)



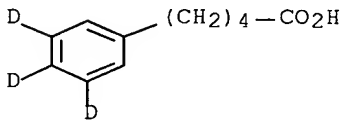
RN 767627-97-4 CAPLUS
CN Benzene-d5-pentanoic-d8 acid (CA INDEX NAME)



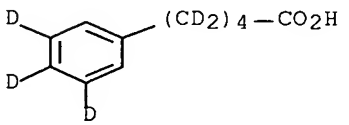
RN 861405-57-4 CAPLUS
CN Benzenepentanoic-d8 acid (9CI) (CA INDEX NAME)



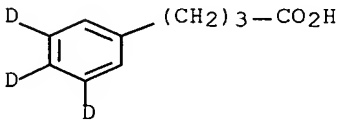
RN 861405-58-5 CAPLUS
CN Benzene-3,4,5-d3-pentanoic acid (9CI) (CA INDEX NAME)



RN 861405-59-6 CAPLUS
CN Benzene-3,4,5-d3-pentanoic-α,α,β,β,γ,γ,.
delta.,δ-d8 acid (9CI) (CA INDEX NAME)



RN 861405-60-9 CAPLUS
CN Benzene-3,4,5-d3-butanoic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:711257 CAPLUS Full-text
DOCUMENT NUMBER: 141:379678
TITLE: Complete Replacement of H2 by D2 via Pd/C-Catalyzed H/D Exchange Reaction
AUTHOR(S): Sajiki, Hironao; Kurita, Takanori; Esaki, Hiroyoshi; Aoki, Fumiyo; Maegawa, Tomohiro; Hirota, Kosaku
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Gifu Pharmaceutical University, Gifu, 502-8585, Japan
SOURCE: Organic Letters (2004), 6(20), 3521-3523
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:379678

AB A general and in situ D2 gas generation method using 10% Pd/C-catalyzed H2-D2 exchange reaction in a H2-D2O system has been developed. H2 gas sealed in a reaction flask was efficiently converted into nearly pure D2 gas, which can be used for the reductive deuteration of substrates possessing reducible functionalities within the mol.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Deuteration**
Deuteration catalysts
Hydrogenation
Hydrogenation catalysts
(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

IT 100-46-9P, Benzylamine, preparation 123-25-1P, Diethyl succinate 4551-39-7P, 2-Deuteriobenzoic acid 4551-62-6P, 4-Deuteriobenzoic acid
782486-40-2P, Benzenepropanoic-α,β-d2 acid-d
782486-42-4P, Benzene-3-d-propanoic acid 782486-43-5P, Benzene-3-d-ethanol
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

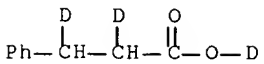
IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

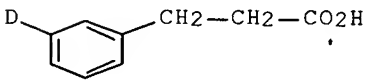
Pd

IT **782486-40-2P**, Benzenepropanoic-α,β-d2 acid-d
782486-42-4P, Benzene-3-d-propanoic acid
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(palladium-catalyzed reductive deuteration using hydrogen and deuterium oxide)

RN 782486-40-2 CAPLUS
CN Benzenepropanoic-α,β-d2 acid-d (9CI) (CA INDEX NAME)



RN 782486-42-4 CAPLUS
CN Benzene-3-d-propanoic acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:589514 CAPLUS Full-text
DOCUMENT NUMBER: 141:139883
TITLE: Method of catalytic deuteration of carbonyl compounds or secondary alcohols by heavy water
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004060831	A1	20040722	WO 2003-JP14182	20031107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2511885	A1	20040722	CA 2003-2511885	20031107
AU 2003277596	A1	20040729	AU 2003-277596	20031107
EP 1577280	A1	20050921	EP 2003-814536	20031107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1732135	A	20060208	CN 2003-80107483	20031107
US 2006116535	A1	20060601	US 2005-539188	20050616
IN 2005KN01449	A	20070720	IN 2005-KN1449	20050726
PRIORITY APPLN. INFO.:			JP 2002-378932 A	20021227

WO 2003-JP14182 W 20031107

OTHER SOURCE(S): CASREACT 141:139883; MARPAT 141:139883

AB Described is a method of deuterating a carbonyl or secondary alc. compound represented by the general formula R1-X-R2 (I) (wherein R1 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aralkyl ; R2 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aryl, aralkyl, alkoxy, aryloxy, hydroxy; X carbonyl, hydroxymethylene), which comprises reacting the compound represented by the general formula I with a deuterium source, in particular D2O, in the presence of a catalyst selected among activated palladium, platinum, rhodium, ruthenium, nickel, and cobalt catalysts. By the method, deuteration, which has been conducted under severe conditions, can be conducted under neutral conditions. Even when the compound contains an unsatd. bond, it can be deuterated without reducing the unsatd. bond. Not only hydrogens near the carbonyl or hydroxymethylene group but also those remotely situated from these groups are selectively deuterated without deuterating the carbon-carbon double or triple bonds. Thus, 500 mg tricyclo[5.2.1.02'6]decan-8-ol and 100 mg Pd-C were suspended in 17 mL D2O, purged with H, and heated at 180° for 24 h in an oil bath to give tricyclo[5.2.1.02'6]decan-8-ol deuterated by 96% at 8-position and 88% at other positions.

IC ICM C07B059-00
ICS C07C029-00; C07C031-02; C07C035-08; C07C035-29; C07C035-37; C07C045-00; C07C049-04; C07C049-08; C07C049-433; C07C049-453; C07C051-00; C07C053-10; C07C053-124; C07C057-04; C07M005-00

CC 21-2 (General Organic Chemistry)

IT **Deuteration**
Deuteration catalysts
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT **7440-02-0**, Raney nickel, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts; catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-16-6D**, Rhodium, supported on alumina **7440-16-6D**, Rhodium, supported on carbon **7440-18-8**, Ruthenium, uses **7440-18-8D**, Ruthenium, supported on carbon **7440-48-4**, Cobalt, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT 79-31-2DP, Isobutyric acid, deuterated 108-93-0DP, Cyclohexanol, deuterated **666-52-4P**, 2-Propanone-1,1,1,3,3,3-d6 13380-89-7DP, Tricyclo[5.2.1.02,6]decan-8-ol, deuterated **14044-94-1P** 18153-61-2DP, Bicyclo[2.2.1]heptan-2-one-3,3-d2, deuterated **21273-02-9DP**, Cyclohexan-1-d-ol, deuterated 51209-49-5P, Cyclohexanone-d10 **53481-06-4P 55935-44-9P** 63870-91-7DP, Norbornenol, deuterated **64118-21-4P** **91468-78-9DP**, Bicyclo[2.2.1]heptan-2-d-2-ol, deuterated **350820-09-6P 725242-18-2P**, 4-Heptanone-d14 725242-19-3DP, deuterated 725242-21-7DP, deuterated **725242-22-8P**, 2-Heptanone-d14 **725242-23-9P**, 3-Heptanone-d14 **725242-24-0P**, 2-Heptanol-d15 **725242-25-1P**, 4-Heptanol-d15 **725242-26-2DP**, deuterated **725242-27-3DP**, deuterated **725242-28-4DP**, deuterated **725242-29-5DP**, deuterated **725242-29-5P 725242-30-8P**

725242-31-9P 725242-32-0DP, deuterated
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT **7440-02-0**, Raney nickel, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts; catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

IT **7440-05-3**, Palladium, uses **7440-05-3D**, Palladium, supported on carbon **7440-06-4**, Platinum, uses **7440-06-4D**, Platinum, supported on carbon **7440-16-6**, Rhodium, uses **7440-16-6D**, Rhodium, supported on alumina **7440-18-8**, Ruthenium, uses **7440-18-8D**, Ruthenium, supported on carbon **7440-48-4**, Cobalt, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

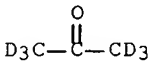
RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

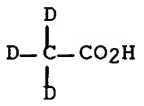
IT **666-52-4P**, 2-Propanone-1,1,1,3,3,3-d6 **14044-94-1P**
21273-02-9DP, Cyclohexan-1-d-ol, deuterated **53481-06-4P**
55935-44-9P 64118-21-4P 91468-78-9DP,
Bicyclo[2.2.1]heptan-2-d-2-ol, deuterated **350820-09-6P**
725242-18-2P, 4-Heptanone-d14 **725242-22-8P**,
2-Heptanone-d14 **725242-23-9P**, 3-Heptanone-d14
725242-24-0P, 2-Heptanol-d15 **725242-25-1P**,
4-Heptanol-d15 **725242-26-2DP**, deuterated **725242-27-3DP**

, deuterated **725242-28-4DP**, deuterated **725242-29-5DP**,
deuterated **725242-29-5P 725242-30-8P**
725242-31-9P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

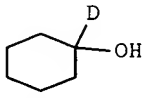
RN 666-52-4 CAPLUS
CN 2-Propanone-1,1,1,3,3,3-d6 (9CI) (CA INDEX NAME)



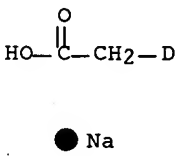
RN 14044-94-1 CAPLUS
CN Acetic-d3 acid, sodium salt (8CI, 9CI) (CA INDEX NAME)



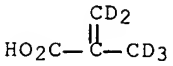
RN 21273-02-9 CAPLUS
CN Cyclohexan-1-d-ol (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



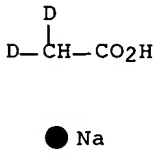
RN 53481-06-4 CAPLUS
CN Acetic-d acid, sodium salt (9CI) (CA INDEX NAME)



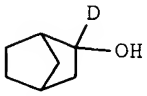
RN 55935-44-9 CAPLUS
CN 2-Propenoic-3,3-d2 acid, 2-(methyl-d3)- (CA INDEX NAME)



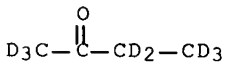
RN 64118-21-4 CAPLUS
CN Acetic-d2 acid, sodium salt (9CI) (CA INDEX NAME)



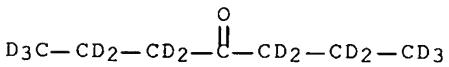
RN 91468-78-9 CAPLUS
CN Bicyclo[2.2.1]heptan-2-d-2-ol (9CI) (CA INDEX NAME)



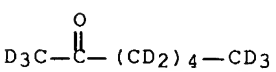
RN 350820-09-6 CAPLUS
CN 2-Butanone-1,1,1,3,3,4,4,4-d8 (9CI) (CA INDEX NAME)



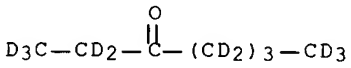
RN 725242-18-2 CAPLUS
CN 4-Heptanone-1,1,1,2,2,3,3,5,5,6,6,7,7,7-d14 (9CI) (CA INDEX NAME)



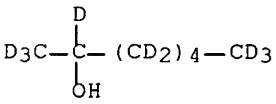
RN 725242-22-8 CAPLUS
CN 2-Heptanone-1,1,1,3,3,4,4,5,5,6,6,7,7,7-d14 (9CI) (CA INDEX NAME)



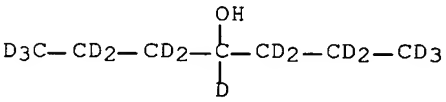
RN 725242-23-9 CAPLUS
CN 3-Heptanone-1,1,1,2,2,4,4,5,5,6,6,7,7,7-d14 (9CI) (CA INDEX NAME)



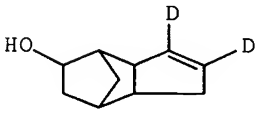
RN 725242-24-0 CAPLUS
CN 2-Heptan-1,1,1,2,3,3,4,4,5,5,6,6,7,7,7-d15-ol (9CI) (CA INDEX NAME)



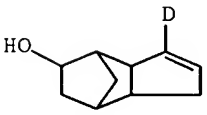
RN 725242-25-1 CAPLUS
CN 4-Heptan-1,1,1,2,2,3,3,4,5,5,6,6,7,7,7-d15-ol (9CI) (CA INDEX NAME)



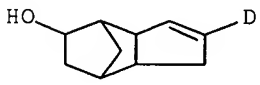
RN 725242-26-2 CAPLUS
CN 4,7-Methano-1H-inden-2,3-d2-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



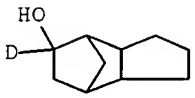
RN 725242-27-3 CAPLUS
CN 4,7-Methano-1H-inden-3-d-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



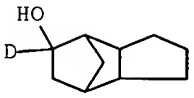
RN 725242-28-4 CAPLUS
CN 4,7-Methano-1H-inden-2-d-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



RN 725242-29-5 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)

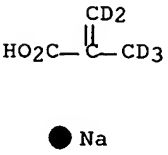


RN 725242-29-5 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



RN 725242-30-8 CAPLUS
CN 4,7-Methano-1H-inden-1,1,2,3,6,7,7-d7-5-ol, octahydro-2,3,3a,4,5,6,7,7a-d8- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 725242-31-9 CAPLUS
CN 2-Propenoic-3,3-d2 acid, 2-(methyl-d3)-, sodium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:453150 CAPLUS Full-text
DOCUMENT NUMBER: 141:23545
TITLE: Method for deuteration or tritiation of heterocyclic compounds
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046066	A1	20040603	WO 2003-JP14181	20031107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2506010	A1	20040603	CA 2003-2506010	20031107
AU 2003277595	A1	20040615	AU 2003-277595	20031107
EP 1561741	A1	20050810	EP 2003-811499	20031107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1714060	A	20051228	CN 2003-80103924	20031107
US 2006025596	A1	20060202	US 2005-534344	20050509
IN 2005KN01145	A	20061110	IN 2005-KN1145	20050615
PRIORITY APPLN. INFO.:			JP 2002-331594 A	20021115
			WO 2003-JP14181 W	20031107

AB A method for deuteration or tritiation of a heterocyclic ring comprises allowing a heterocyclic compound to be present under a sealing and refluxing condition in a deuterated or tritiated solvent (e.g., D2O) in the presence of an activated catalyst selected from among a palladium catalyst, a platinum catalyst, a rhodium catalyst, a ruthenium catalyst, a nickel catalyst and a cobalt catalyst. The method allows a deuteration or tritiation temperature to be kept at a temperature higher than the boiling temperature of the solvent, which results in the replacement of a hydrogen atom in a heterocyclic ring of a heterocyclic compound with very good efficiency. Further, the method can be widely used for the deuteration or tritiation of various types of heterocyclic compds. in a com. process.

IC ICM C07B059-00
ICS C07D209-08; C07D209-20; C07D213-06; C07D231-12; C07D233-58; C07D235-08; C07D239-47; C07D239-54; C07D471-04; C07D473-30; C07D473-34; C07H019-067; C07H019-167; C07M005-00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 26, 33, 34
IT **Deuteration**
Tritiation
(method for deuteration or tritiation of heterocyclic compds.)
IT **Deuteration catalysts**
Tritiation catalysts
(palladium and platinum, in method for deuteration or tritiation of

heterocyclic compds.)
IT **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses
7440-06-4, Platinum, uses **7440-16-6**, Rhodium, uses
7440-18-8, Ruthenium, uses 7440-44-0, Carbon, uses
7440-48-4, Cobalt, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(method for deuteration or tritiation of heterocyclic compds.)
IT 4166-68-1P 6745-43-3P, 1H-Imidazole-2,4,5-d3 22194-79-2P
24897-52-7P, 2,4(1H,3H)-Pyrimidinedione-5,6-d2 **40632-21-1P**,
Uridine-5,6-d2 62595-11-3P, L-Tryptophan-2,4,5,6,7-d5
82845-88-3P, Adenosine-2,8-d2 **96412-41-8P**, Guanosine-8-d
106391-24-6P 130317-91-8P 200496-79-3P 350818-65-4P 697806-98-7P
697806-99-8P 697807-00-4P, 1H-Purin-2,8-d2-6-amine **697807-01-5P**
, Inosine-2,8-d2 697807-02-6P 697807-03-7P 697807-04-8P
697807-05-9P 697807-06-0P 697807-07-1P
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(method for deuteration or tritiation of heterocyclic compds.)
IT **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses
7440-06-4, Platinum, uses **7440-16-6**, Rhodium, uses
7440-18-8, Ruthenium, uses **7440-48-4**, Cobalt, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(method for deuteration or tritiation of heterocyclic compds.)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

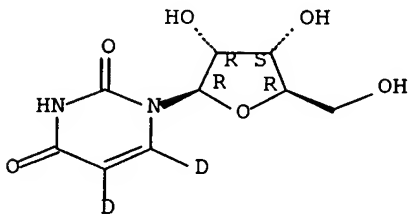
Ru

RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

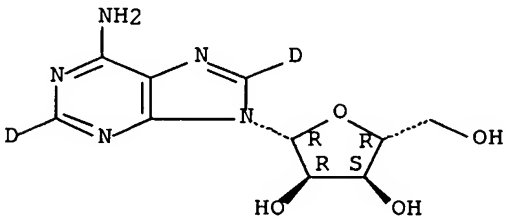
IT **40632-21-1P**, Uridine-5,6-d2 **82845-88-3P**, Adenosine-2,8-d2 **96412-41-8P**, Guanosine-8-d **697807-01-5P**, Inosine-2,8-d2
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(method for deuteration or tritiation of heterocyclic compds.)
RN 40632-21-1 CAPLUS
CN Uridine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



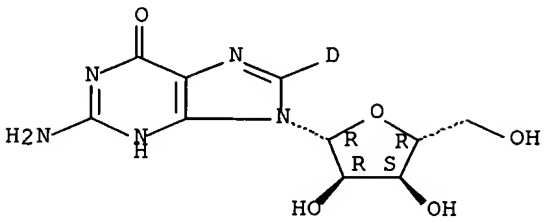
RN 82845-88-3 CAPLUS
CN Adenosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



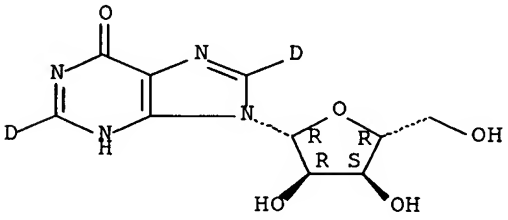
RN 96412-41-8 CAPLUS
CN Guanosine-8-d (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 697807-01-5 CAPLUS
CN Inosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:231394 CAPLUS Full-text
DOCUMENT NUMBER: 140:406566
TITLE: Palladium-catalyzed H-D exchange reaction under hydrothermal condition
AUTHOR(S): Matsubara, Seijiro; Yokota, Yutaka; Oshima, Koichiro
CORPORATE SOURCE: Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, 615-8510, Japan
SOURCE: Chemistry Letters (2004), 33(3), 294-295
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:406566

AB Alkenes and alkanes were converted into fully deuterium labeled ones by treatment with palladium on charcoal and deuterium oxide under hydrothermal condition. This simple method to get fully deuterium labeled compds. is easy to apply to various types of organic compds.

CC 24-6 (Alicyclic Compounds)
IT **Deuteration**
Deuteration catalysts
(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)
IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)

IT 1486-01-7P 10249-89-5P, Cyclooctene-d14 16450-78-5P, Cyclododecane-d24
36340-20-2P, Pentadecane-d32 688320-41-4P 688320-42-5P,
Cyclopentadecane-d30 688320-43-6P, Cyclooctanone-d14 688320-44-7P,
Cyclodecanone-d18 688320-45-8P, Cyclododecanone-d22 688320-46-9P,
Cyclopentadecanone-d28 **688320-48-1P** 688320-49-2P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)

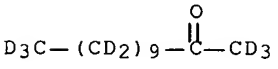
IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

Pd

IT **688320-48-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(palladium-catalyzed H-D exchange reaction under hydrothermal conditions)

RN 688320-48-1 CAPLUS
CN 2-Dodecanone-1,1,1,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-d24 (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:991461 CAPLUS Full-text
DOCUMENT NUMBER: 140:41620
TITLE: Process for deuteration of inert methylene
INVENTOR(S): Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003104166	A1	20031218	WO 2002-JP11785		20021112
W: JP, US					
US 2005177015	A1	20050811	US 2004-516638		20041202
US 7126023	B2	20061024			
PRIORITY APPLN. INFO.:			JP 2002-166224	A	20020606
			WO 2002-JP11785	W	20021112

OTHER SOURCE(S): MARPAT 140:41620

AB The invention relates to a process for deuteration of inert alkanes with activated palladium-carbon, specifically, a process for deuterating a compound having either a Me group or an alkylene group having two or more carbon atoms in a state directly bonded to an optionally substituted aromatic ring through replacement of one or more hydrogen atoms of the Me group or one or more of the benzylic and other hydrogen atoms of the alkylene group by deuterium, characterized in that the above compound is subjected to refluxing in a closed system in the presence of activated palladium-carbon in a state dissolved in a deuterated solvent.

IC ICM C07B059-00
ICS C07M005-00

CC 21-2 (General Organic Chemistry)

IT **Deuteration**
Deuteration catalysts
(process for deuteration of inert methylene using activated palladium-carbon catalyst)

IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(carbon-supported; process for deuteration of inert methylene using activated palladium-carbon catalyst)

IT 1124-18-1P 14202-49-4P 38729-11-2P 65087-58-3P 94367-56-3P
117637-87-3P, Benzenepropan-β,β,γ,γ-d4-ol
156310-21-3P **634897-72-6P** 634897-76-0P 634897-78-2P
634897-80-6P 634897-82-8P 634897-84-0P **634897-86-2P**,
Benzenepropanoic-d4 acid-d **634897-88-4P**, Benzene-d5-butanoic-d6 acid-d **634897-90-8P 634897-92-0P 634897-99-7P**
634898-02-5P, Benzenebutan-β,β,γ,γ,δ,δ-d6-ol 634898-04-7P, Benzenepentan-β,β,γ,γ,δ,δ,ε,ε-d8-ol 634898-08-1P 634898-10-5P
634898-14-9P 634898-16-1P 634898-20-7P 634898-23-0P 634898-25-2P
634898-29-6P 634898-34-3P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for deuteration of inert methylene using activated palladium-carbon catalyst)

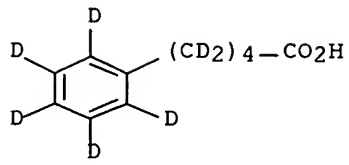
IT **7440-05-3**, Palladium, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(carbon-supported; process for deuteration of inert methylene using activated palladium-carbon catalyst)

RN 7440-05-3 CAPLUS
CN Palladium (CA INDEX NAME)

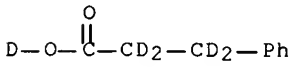
Pd

IT **634897-72-6P 634897-86-2P**, Benzenepropanoic-d4 acid-d
634897-88-4P, Benzene-d5-butanoic-d6 acid-d **634897-90-8P 634897-92-0P 634897-99-7P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for deuteration of inert methylene using activated palladium-carbon catalyst)

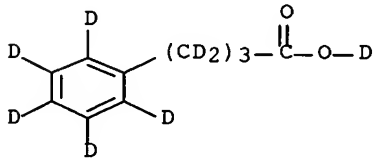
RN 634897-72-6 CAPLUS
CN Benzene-d5-pentanoic-d8 acid, sodium salt (9CI) (CA INDEX NAME)



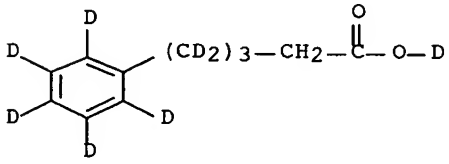
RN 634897-86-2 CAPLUS
CN Benzenepropanoic-d4 acid-d (9CI) (CA INDEX NAME)



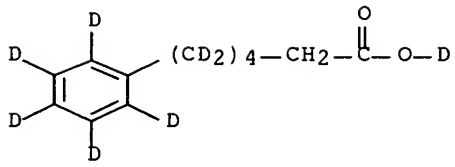
RN 634897-88-4 CAPLUS
CN Benzene-d5-butanoic-d6 acid-d (9CI) (CA INDEX NAME)



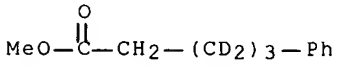
RN 634897-90-8 CAPLUS
CN Benzene-d5-pentanoic-β,β,γ,γ,δ,δ-d6 acid-d (9CI) (CA INDEX NAME)



RN 634897-92-0 CAPLUS
CN Benzene-d5-hexanoic-β,β,γ,γ,δ,δ,.epsilon.,ε-d8 acid-d (9CI) (CA INDEX NAME)



RN 634897-99-7 CAPLUS
CN Benzenepentanoic-β,β,γ,γ,δ,δ-d6 acid, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:474175 CAPLUS Full-text
DOCUMENT NUMBER: 139:395665
TITLE: Combining microwave-enhanced deuteration reactions with parallel synthesis procedures
AUTHOR(S): Chappelle, Michael R.; Harding, John R.; Kent, Barry B.; Jones, John R.; Lu, Shui-Yu; Morgan, Alan D.
CORPORATE SOURCE: Amersham Biosciences, The Maynard Centre, Cardiff, CF14 7YT, UK
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 567-574
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:395665

AB The development of combined microwave-enhanced/parallel synthesis procedures and their application to the deuteration of organic compds. via examples of solid-state hydrogenation is reported. Other labeling procedures, such as solution state catalytic dehalogenations, hydrogenations as well as hydrogen isotope exchange reactions also benefit from the combined technol.

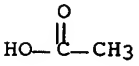
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT Debromination
Dechlorination
Dehalogenation
Deuteration catalysts
Microwave
Solid phase synthesis
(combining microwave-enhanced deuteration with parallel synthesis procedures)
IT **Deuteration**
Hydrogenation catalysts
(solid-state deuteration; combining microwave-enhanced deuteration with parallel synthesis procedures)
IT **3375-31-3 10049-07-7,** Rhodium chloride (RhCl3)

RL: **CAT (Catalyst use)**; USES (Uses)
(combining microwave-enhanced deuteration with parallel synthesis procedures)

IT 10473-16-2P 16089-48-8P, 3-Phenyl-2-Propenoic acid potassium salt 36568-19-1P, 3-(4-Chlorophenyl)-2-Propenoic acid potassium salt 625383-67-7P, 3-(4-Bromophenyl)-2-propenoic acid potassium salt 625383-68-8P, 4-Bromobenzenepropanoic-α,β-d2 acid potassium salt **625383-69-9P**, 3-(Phenyl-4-d)-2-Propenoic acid potassium salt 625383-70-2P, 3-(3-Bromophenyl)-2-propenoic acid potassium salt 625383-72-4P **625383-73-5P**, 3-(Phenyl-3-d)-2-Propenoic acid potassium salt 625383-74-6P, 1-Bromo-4-(ethyl-1,2-d2)benzene 625383-75-7P, 3-(4-Fluorophenyl)-2-Propenoic acid potassium salt 625383-76-8P, 3-(2-Chlorophenyl)-2-Propenoic acid potassium salt 625383-77-9P, 3-(3-Chlorophenyl)-2-Propenoic acid potassium salt **625383-78-0P** 625383-80-4P, 4-Fluorobenzenepropanoic-α,β-d2 acid potassium salt 625383-82-6P, 2-Chlorobenzenepropanoic-α,β-d2 acid potassium salt 625383-84-8P, 3-Chlorobenzenepropanoic-α,β-d2 acid potassium salt 625383-86-0P, 4-Chlorobenzenepropanoic-α,β-d2 acid potassium salt 625383-88-2P, 1-Bromo-4-(ethenyl-1,2-d2)benzene 625383-90-6P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(combining microwave-enhanced deuteration with parallel synthesis procedures)

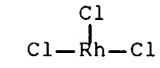
IT **3375-31-3 10049-07-7**, Rhodium chloride (RhCl3)
RL: **CAT (Catalyst use)**; USES (Uses)
(combining microwave-enhanced deuteration with parallel synthesis procedures)

RN 3375-31-3 CAPLUS
CN Acetic acid, palladium(2+) salt (2:1) (CA INDEX NAME)



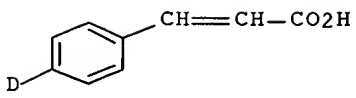
●1/2 Pd(II)

RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)

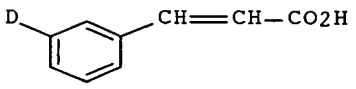


IT **625383-69-9P**, 3-(Phenyl-4-d)-2-Propenoic acid potassium salt
625383-73-5P, 3-(Phenyl-3-d)-2-Propenoic acid potassium salt
625383-78-0P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(combining microwave-enhanced deuteration with parallel synthesis procedures)

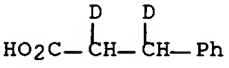
RN 625383-69-9 CAPLUS
CN 2-Propenoic acid, 3-(phenyl-4-d)-, potassium salt (9CI) (CA INDEX NAME)



RN 625383-73-5 CAPLUS
CN 2-Propenoic acid, 3-(phenyl-3-d)-, potassium salt (9CI) (CA INDEX NAME)



RN 625383-78-0 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, potassium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:483457 CAPLUS Full-text
DOCUMENT NUMBER: 138:4188
TITLE: Development of combined microwave-enhanced labelling procedures for maximizing deuterium incorporation
AUTHOR(S): Chapelle, Michael R.; Kent, Barry B.; Jones, John R.; Lu, Shui-Yu; Morgan, Alan D.
CORPORATE SOURCE: Amersham Plc, Cardiff Laboratories, Cardiff, CF14 7YT, UK
SOURCE: Tetrahedron Letters (2002), 43(29), 5117-5118
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:4188

AB Combined hydrogenation/aromatic dehalogenation under microwave-enhanced conditions provides a rapid route to deuterium labeled compds. with enhanced isotopic incorporation.

CC 21-2 (General Organic Chemistry)

IT Debromination
Debromination catalysts
Dechlorination
Dechlorination catalysts
Deuteration
Deuteration catalysts
Hydrogenation
Hydrogenation catalysts
Microwave
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via rhodium- and palladium-catalyzed microwave-induced combined hydrogenation/aromatic dehalogenation procedure)

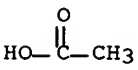
IT **3375-31-3,** Palladium diacetate **10049-07-7,** Rhodium chloride (RhCl3)
RL: **CAT (Catalyst use);** USES (Uses)
(microwave-induced rhodium- and palladium-catalyzed combined hydrogenation/aromatic dehalogenation routes for preparation of deuterium-labeled compds. with enhanced isotopic incorporation)

IT **99532-30-6P** 477284-15-4P **477284-16-5P,** Benzene-4-d-propanoic-α,β-d2 acid
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via combined microwave-induced hydrogenation/aromatic dehalogenation procedure)

IT **477284-17-6P,** Benzene-3-d-propanoic-α,β-d2 acid
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via microwave-induced hydrogenation/aromatic dehalogenation procedure)

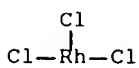
IT **3375-31-3,** Palladium diacetate **10049-07-7,** Rhodium chloride (RhCl3)
RL: **CAT (Catalyst use);** USES (Uses)
(microwave-induced rhodium- and palladium-catalyzed combined hydrogenation/aromatic dehalogenation routes for preparation of deuterium-labeled compds. with enhanced isotopic incorporation)

RN 3375-31-3 CAPLUS
CN Acetic acid, palladium(2+) salt (2:1) (CA INDEX NAME)

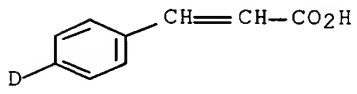


●1/2 Pd(II)

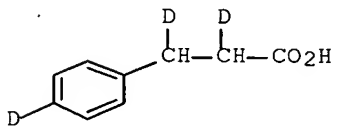
RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)



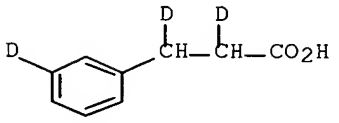
IT **99532-30-6P 477284-16-5P,** Benzene-4-d-propanoic-α,β-d2 acid
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via combined microwave-induced hydrogenation/aromatic dehalogenation procedure)
RN 99532-30-6 CAPLUS
CN 2-Propenoic acid, 3-(phenyl-4-d)- (9CI) (CA INDEX NAME)



RN 477284-16-5 CAPLUS
CN Benzene-4-d-propanoic-α,β-d2 acid (9CI) (CA INDEX NAME)



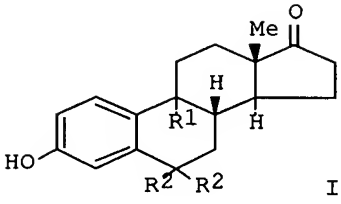
IT **477284-17-6P,** Benzene-3-d-propanoic-α,β-d2 acid
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via microwave-induced hydrogenation/aromatic dehalogenation procedure)
RN 477284-17-6 CAPLUS
CN Benzene-3-d-propanoic-α,β-d2 acid (9CI) (CA INDEX NAME)



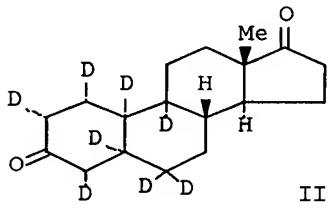
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:550049 CAPLUS Full-text
DOCUMENT NUMBER: 133:322037
TITLE: Deuteration of estrogens using Pd/C as a catalyst
AUTHOR(S): Kiuru, Paula; Wahala, Kristiina
CORPORATE SOURCE: Department of Chemistry, Organic Chemistry Laboratory,

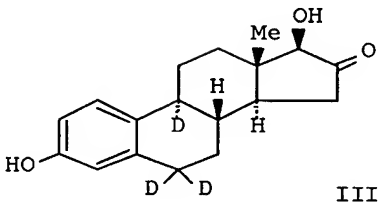
University of Helsinki, FIN-00014, Finland
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 475-477. Editor(s): Heys, J. Richard; Melillo, David G. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69AGFQ
DOCUMENT TYPE: Conference
LANGUAGE: English
GI



I



II



III

AB The reduction of estrone (I; R1 = R2 = H) using D2 on Pd/C gives 1α,2α,4α,5α,6,6,9α,10α-[2H3]estrane- 3,17-dione (II), the configuration of deuteriums been established by NMR. Pd/C catalyzes the H-D exchange also at the benzylic positions of estrogens. 6,6,9-[2H3]estrone (I; R1 = R2 = D) and 6,6,9-[2H3]-16- ketoestradiol (III) were synthesized in high isotopic purity.

CC 32-3 (Steroids)

IT Absolute configuration
Deuteration
Deuteration catalysts
(stereoselective deuteration of estrogens using palladium/carbon as a catalyst)

IT **7440-05-3D**, Palladium, on carbon, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(stereoselective deuteration of estrogens using palladium/carbon as a catalyst)

IT 50888-33-0P, 6,6,9-[2H3]Estrone 303128-11-2P, 1α,5α,6,6,9α,10α-[2H6]Estrane-3,17-dione
303128-12-3P, 6,6,9-[2H3]-16-Ketoestradiol
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(stereoselective deuteration of estrogens using palladium/carbon as a catalyst)

IT **7440-05-3D**, Palladium, on carbon, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(stereoselective deuteration of estrogens using palladium/carbon as a catalyst)

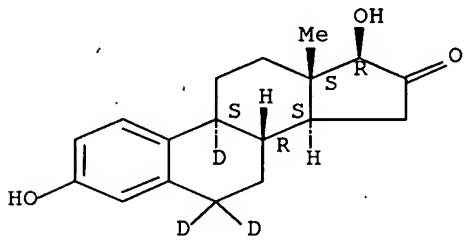
RN 7440-05-3 CAPLUS

CN Palladium (CA INDEX NAME)

Pd

IT **303128-12-3P**, 6,6,9-[2H3]-16-Ketoestradiol
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(stereoselective deuteration of estrogens using palladium/carbon as a catalyst)
RN 303128-12-3 CAPLUS
CN Estra-1,3,5(10)-trien-16-one-6,6,9-d3, 3,17-dihydroxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:549991 CAPLUS Full-text
DOCUMENT NUMBER: 134:147329
TITLE: Convenient synthesis of deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide
AUTHOR(S): Tsuzuki, Hirohisa; Mataka, Shuntaro; Tashiro, Masashi
CORPORATE SOURCE: Center of Advanced Instrumental Analysis, Kyusha University, Kasuga, 816, Japan
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 203-206. Editor(s): Heys, J. Richard; Melillo, David G. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69AGFQ
DOCUMENT TYPE: Conference
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:147329
AB A symposium report on the deuteration of polyhalophenolic substrates in the presence of nickel-aluminum alloy.
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 34
IT **Deuteration**
Deuteration catalysts
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum

alloy in alkaline deuterium oxide)

IT **11114-68-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)

IT **77787-72-5P 93131-17-0P**, Cyclohexan-d11-ol
324520-34-5P 324520-35-6P 324520-36-7P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)

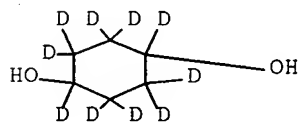
IT **11114-68-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)

RN 11114-68-4 CAPLUS
CN Aluminum alloy, nonbase, Al,Ni (CA INDEX NAME)

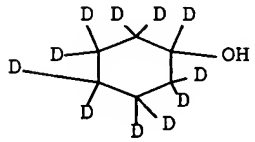
Component	Component Registry Number
Al	7429-90-5
Ni	7440-02-0

IT **77787-72-5P 93131-17-0P**, Cyclohexan-d11-ol
324520-34-5P 324520-35-6P 324520-36-7P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)

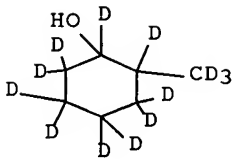
RN 77787-72-5 CAPLUS
CN 1,4-Cyclohexane-1,2,2,3,3,4,5,5,6,6-d10-diol (9CI) (CA INDEX NAME)



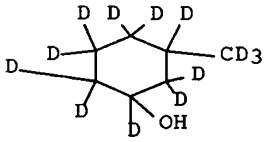
RN 93131-17-0 CAPLUS
CN Cyclohexan-d11-ol (9CI) (CA INDEX NAME)



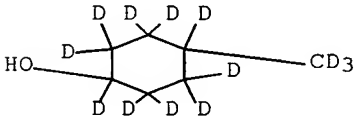
RN 324520-34-5 CAPLUS
CN Cyclohexan-1,2,2,3,3,4,4,5,5,6-d10-ol, 6-(methyl-d3)- (9CI) (CA INDEX NAME)



RN 324520-35-6 CAPLUS
CN Cyclohexan-1,2,2,3,3,4,4,5,6,6-d10-ol, 5-(methyl-d3)- (9CI) (CA INDEX NAME)



RN 324520-36-7 CAPLUS
CN Cyclohexan-1,2,2,3,3,4,5,5,6,6-d10-ol, 4-(methyl-d3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:414551 CAPLUS Full-text
DOCUMENT NUMBER: 133:192893
TITLE: Multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst
AUTHOR(S): Papp, Eva; Banyai, Istvan; Joo, Ferenc
CORPORATE SOURCE: Research Group of Homogeneous Catalysis, Hungarian Academy of Sciences, Debrecen, H-4010, Hung.
SOURCE: Reaction Kinetics and Catalysis Letters (2000), 69(1), 23-30
CODEN: RKCLAU; ISSN: 0304-4122
PUBLISHER: Akademiai Kiado
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hydrogenations in aqueous systems with the soluble [Pd(alizarin monosulfonate)2] catalyst resulted in extensive deuteration of crotonic, trans-2-pentenoic and itaconic acids regardless of whether the deuterium source was D2 or D2O. Itaconic acid was deuterated up to 3.6 D/methylsuccinic

acid. Detailed 1H-and 13C-NMR studies identified six isotopomers of the deuterated methylsuccinic acid product and revealed an important role of the H/D exchange on the catalytically active Pd-intermediate.

CC 23-16 (Aliphatic Compounds)

IT **Deuteration**
Deuteration catalysts
Hydrogenation
Hydrogenation catalysts
(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst)

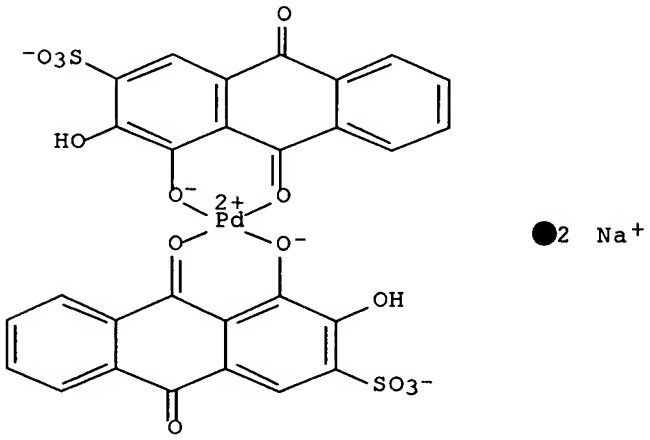
IT **74091-55-7**
RL: **CAT (Catalyst use)**; USES (Uses)
(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst)

IT 498-21-5P 169127-02-0P **289679-94-3P**, Butanoic-d acid **289679-95-4P**, Pentanoic-d acid 289679-96-5P 289679-97-6P 289679-98-7P 289679-99-8P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst)

IT **74091-55-7**
RL: **CAT (Catalyst use)**; USES (Uses)
(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst)

RN 74091-55-7 CAPLUS

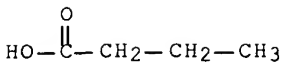
CN Palladate(2-), bis[9,10-dihydro-3-hydroxy-4-(hydroxy-κO)-9-oxo-10-(oxo-κO)-2-anthracenesulfonato(2-)]-, disodium (9CI) (CA INDEX NAME)



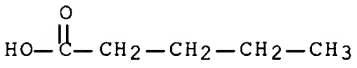
IT **289679-94-3P**, Butanoic-d acid **289679-95-4P**, Pentanoic-d acid
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(hydrogenation and multiple deuteration of water-soluble olefinic acids with a [Pd(alizarin monosulfonate)2] catalyst)

RN 289679-94-3 CAPLUS

CN Butanoic-d acid (9CI) (CA INDEX NAME)



RN 289679-95-4 CAPLUS
CN Pentanoic-d acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:324308 CAPLUS Full-text
DOCUMENT NUMBER: 127:17291
TITLE: First Evidence That the Mechanism of Catalytic Hydrogenation with Homogeneous Palladium and Rhodium Catalysts Is Strongly Influenced by Substrate Polarity
AUTHOR(S): Yu, Jinquan; Spencer, Jonathan B.
CORPORATE SOURCE: University Chemical Laboratory, University of Cambridge, Cambridge, CB2 1EW, UK
SOURCE: Journal of the American Chemical Society (1997), 119(22), 5257-5258
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have observed that when cis-alkenes are hydrogenated with homogeneous palladium and rhodium catalysts they readily isomerize to the trans-configuration with the incorporation of a deuterium atom. By studying how electron withdrawing and donating groups conjugated to the double bond influence the location of deuterium addition we have been able to gain a clear insight into how the metal hydrogen bond in the catalyst is polarized just prior to adding to the cis-alkene. Remarkably, the result demonstrate that the palladium hydrogen bond is capable of being polarized in either mode (a Pdδ+-Hδ- or b Pdδ--Hδ+) depending on the coulombic properties of the substrate, whereas the rhodium catalyst studied is dominated by mode a (Rhδ+-Hδ-). This provides strong evidence that the mechanism of catalytic hydrogenation is a 2 electron process that can be dramatically affected by the substrate's polarity.

CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 29, 67
IT Conjugation (bond)
Deuteration
Deuteration catalysts
Electron transfer
Hydrogenation
Hydrogenation catalysts
Isomerization
Isomerization catalysts
NMR (nuclear magnetic resonance)
Regiochemistry

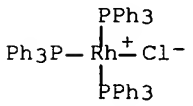
Resonance
Substituent effects
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

IT **14694-95-2**, Chlorotris(triphenylphosphine)rhodium
31277-98-2, Bis[1,2-bis(diphenylphosphino)ethane]palladium
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

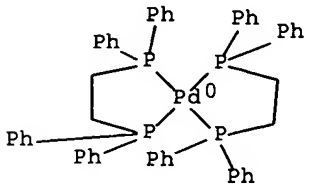
IT 107-93-7P 140-10-3P, preparation 623-43-8P 943-89-5P 1005-64-7P 1011-54-7P 4747-15-3P **69104-43-4P** 89039-12-3P 89039-13-4P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

IT **14694-95-2**, Chlorotris(triphenylphosphine)rhodium
31277-98-2, Bis[1,2-bis(diphenylphosphino)ethane]palladium
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)

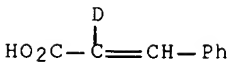


RN 31277-98-2 CAPLUS
CN Palladium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]-, (T-4)- (9CI) (CA INDEX NAME)



IT **69104-43-4P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)

RN 69104-43-4 CAPLUS
CN 2-Propenoic-2-d acid, 3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:98985 CAPLUS Full-text
DOCUMENT NUMBER: 124:260517
TITLE: Retention of optical purity in H-D exchange reactions catalyzed by cobalt-aluminum alloy in Na2CO3-D2O
AUTHOR(S): Mukumoto, Mamoru; Tsuzuki, Hirohisa; Mataka, Shuntaro; Tashiro, Masashi; Tsukinoki, Takehito; Nagano, Yoshiaki
CORPORATE SOURCE: Dep. Mol. Sci. Technol., Kyushu Univ., Kasuga, 816, Japan
SOURCE: Chemistry Letters (1996), (2), 165-6
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:260517

AB Co-Al alloy in a sodium carbonate-deuterium oxide solution catalyzes the H-D exchange reaction of optically active benzylic hydrogen atom without racemization. Thus, (R)-mandelic acid give Me α-D-(R)-mandelate in 89% yield with 99% enantiomeric excess.

CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Deuteration catalysts**
(stereoselective; deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)
IT **Deuteration**
(stereoselective, deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)
IT **11114-55-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)
IT 175289-31-3P **175289-32-4P** 175289-33-5P 175289-34-6P
175289-35-7P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)
IT **11114-55-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)
RN 11114-55-9 CAPLUS
CN Aluminum alloy, nonbase, Al,Co (CA INDEX NAME)

Component	Component Registry Number
Al	7429-90-5
Co	7440-48-4

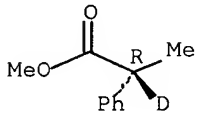
IT **175289-32-4P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)

RN 175289-32-4 CAPLUS

CN Benzeneacetic-d acid, α-methyl-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:231056 CAPLUS Full-text
DOCUMENT NUMBER: 110:231056
TITLE: Homogeneous deuteration of alkenes using [RhCl(4R,5R-diop)] catalysts
AUTHOR(S): Gungor, Muammer; Jardine, Fred H.; Wheatley, J. Denis
CORPORATE SOURCE: Dep. Phys. Sci., North East London Polytech., London, E15 4LZ, UK
SOURCE: Polyhedron (1988), 7(19-20), 1827-9
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mass spectrometric analyses of the products from the homogeneous deuteration of alkenes using the title (4R,5R- DIOP)/{[RhCl(cyclooctene)2]2} catalyst system show that considerable quantities of polydeuterated products are obtained. These products arise from the decomposition of the intermediate rhodium(III)alkyl complex [RhDCl(alkyl)(DIOP)] before the second atom of deuterium can be transferred to the alkyl ligand. Its decomposition by β-hydride abstraction brings about both polydeuteration and scrambled addition of deuterium to the alkene. The yields of specifically deuterated products are inferior to those obtained from Wilkinson-type catalysts. The best yields of dideuterated products are obtained from substituted alkenes that chelate to the catalyst and thereby stabilize the intermediate alkyl. The preparation of a threitol ditosylate intermediate in dry pyridine was noted for its dangerous exothermicity.

CC 23-2 (Aliphatic Compounds)
Section cross-reference(s): 24, 25

IT **Deuteration**
(of alkenes, mechanism of catalytic)

IT **Deuteration catalysts**
(rhodium-DIOP complex, for alkenes)

IT **12279-09-3**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, containing DIOP, for deuteration of alkenes)

IT **66502-82-7P**
RL: PRP (Properties); **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and carbon-13 NMR of)

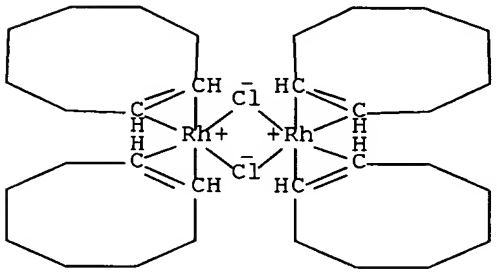
IT 292-64-8P, Cyclooctane 24588-43-0P, Octane-1,2-d2 33283-80-6P, Bicyclo[2.2.1]heptane-2,3-d2 71501-04-7P, Octane-d 73811-48-0P 86812-02-4P, Cyclooctane-d 92475-64-4P, Hexane-1,2-d2 95236-97-8P, Heptane-1,2-d2 95237-00-6P 98821-91-1P, Cyclohexane-1,2-d2

118296-70-1P, Octane-1,2,?-d3 118296-71-2P, Octane-1,2,?,?-d4
118297-06-6P 118297-07-7P 118297-11-3P, Heptane-d 118297-12-4P,
Heptane-1,2,?-d3 118297-17-9P, Hexane-1,2,?-d3 118297-18-0P,
Hexane-1,2,?,?-d4 120625-93-6P, Cyclohexanone-2,3-d2 120625-94-7P,
Cyclooctane-1,2-d2 120625-95-8P 120625-96-9P **120625-97-0P,**
2-Hexanone-5,6-d2 120625-98-1P, Cyclohexane-1,2,?-d3 120625-99-2P,
Cyclohexanone-2,3,?-d3 120626-00-8P, Cyclooctane-1,2,?-d3 120626-01-9P
120626-02-0P **120626-03-1P** 120626-04-2P, Cyclooctane-1,2,?,?-d4
120626-05-3P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

IT **12279-09-3**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, containing DIOP, for deuteration of alkenes)

RN 12279-09-3 CAPLUS

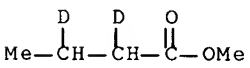
CN Rhodium, di-μ-chlorotetrakis[(1,2-η)-cyclooctene]di- (CA INDEX NAME)



IT **66502-82-7P**
RL: PRP (Properties); **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and carbon-13 NMR of)

RN 66502-82-7 CAPLUS

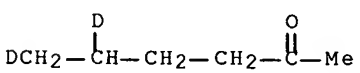
CN Butanoic-2,3-d2 acid, methyl ester (CA INDEX NAME)



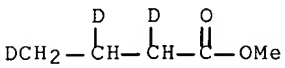
IT **120625-97-0P**, 2-Hexanone-5,6-d2 **120626-03-1P**
120626-05-3P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

RN 120625-97-0 CAPLUS

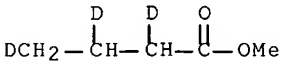
CN 2-Hexanone-5,6-d2 (9CI) (CA INDEX NAME)



RN 120626-03-1 CAPLUS
CN Butanoic-2,3,4-d3 acid, methyl ester (9CI) (CA INDEX NAME)



RN 120626-05-3 CAPLUS
CN Butanoic-2,3,4,?-d4 acid, methyl ester (9CI) (CA INDEX NAME)



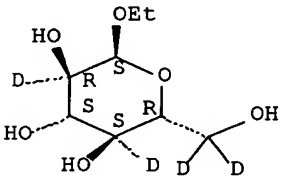
L19 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:545159 CAPLUS Full-text
DOCUMENT NUMBER: 97:145159
ORIGINAL REFERENCE NO.: 97:24193a,24196a
TITLE: Some stereochemical characteristics of C-1H-C-2H exchange-reactions with Raney nickel catalyst in deuterium oxide
AUTHOR(S): Balza, Felipe; Perlin, Arthur S.
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, H3C 3G1, Can.
SOURCE: Carbohydrate Research (1982), 107(2), 270-8
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In C-deuteration of carbohydrates with Raney Ni in D2O, the following reaction-characteristics were observed: (a) at least 2 OH groups, not necessarily contiguous, are required for 1H-2H exchange to occur; (b) the rate of isotope incorporation into alkyl glycopyranosides is relatively slow when the C-H bond undergoing exchange is syn-axial with respect to an alkoxy group or when the bond is axial and vicinal to an equatorial alkoxyl group; (c) an increase in the size of the alkoxyl substituent leads to further diminution in the rate of exchange; (d) an equatorial H atom undergoes exchange more readily than an axial one; and (e) isotope exchange proceeds primarily with retention of configuration, although some degree of isomerization is almost always observed
CC 33-1 (Carbohydrates)
Section cross-reference(s): 22
IT **Deuteration catalysts**
(nickel, for carbohydrates)
IT **Deuteration**
(of carbohydrates over Raney nickel)
IT **7440-02-0**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for deuteration of carbohydrates)
IT 68922-38-3P **83158-38-7P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
IT **7440-02-0**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)

(catalysts, for deuteration of carbohydrates)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

IT **83158-38-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 83158-38-7 CAPLUS
CN α-D-Glucopyranoside-2,4,6,6-C-d4, ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



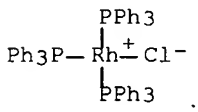
L19 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:461411 CAPLUS Full-text
DOCUMENT NUMBER: 95:61411
ORIGINAL REFERENCE NO.: 95:10371a,10374a
TITLE: A versatile procedure for the preparation of palmitic acid-d2 and stearic acid-d6
AUTHOR(S): Adlof, R. O.; Emken, E. A.
CORPORATE SOURCE: North. Reg. Res. Cent., USDA, Peoria, IL, 61604, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1981), 18(3), 419-26
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:61411
AB Me(CH2)3(CD2)2(CHD)2(CH2)7CO2H and Me(CH2)5(CHD)2(CH2)7CO2H were prepared from the corresponding 9,10-unsatd. Me esters by catalytic deuteration [(Ph3P)3RhCl, C6H6, under D, overnight) and saponification (KOH, aqueous MeOH, under N, reflux, 1.5). Me(CH2)5CH:CH(CH2)7CO2Me was prepared (65%) by Wittig reaction of [Me(CH2)6Ph3P]+I- with OHC(CH2)7CO2Me (DMF, NaOMe, 11°, overnight).
CC 23-16 (Aliphatic Compounds)
IT **Deuteration**
(of unsatd. fatty acid esters, rhodium-catalyzed)
IT **Deuteration catalysts**
(tris(triphenylphosphine)chlororhodium, for unsatd. fatty acids)
IT **14694-95-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for deuteration of unsatd. fatty acids)
IT **78387-67-4P 78387-69-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP**

(Preparation); RACT (Reactant or reagent)
(preparation and saponification of)

IT **78387-68-5P 78387-70-9P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

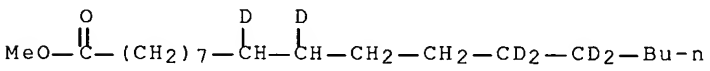
IT **14694-95-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for deuteration of unsatd. fatty acids)

RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)

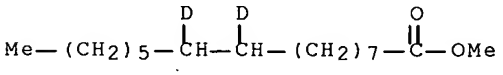


IT **78387-67-4P 78387-69-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and saponification of)

RN 78387-67-4 CAPLUS
CN Octadecanoic-9,10,13,13,14,14-d6 acid, methyl ester (9CI) (CA INDEX NAME)

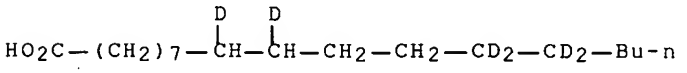


RN 78387-69-6 CAPLUS
CN Hexadecanoic-9,10-d2 acid, methyl ester (9CI) (CA INDEX NAME)

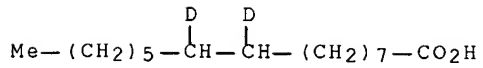


IT **78387-68-5P 78387-70-9P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

RN 78387-68-5 CAPLUS
CN Octadecanoic-9,10,13,13,14,14-d6 acid (9CI) (CA INDEX NAME)



RN 78387-70-9 CAPLUS
CN Hexadecanoic-9,10-d2 acid (9CI) (CA INDEX NAME)



L19 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:139371 CAPLUS Full-text
DOCUMENT NUMBER: 86:139371
ORIGINAL REFERENCE NO.: 86:21873a,21876a
TITLE: Molecular hydrogenation, deuteration and oxygenation
AUTHOR(S): Khan, N. A.; Ahmed, R.
CORPORATE SOURCE: BCSIR Lab., Chittagong, Bangladesh
SOURCE: Bangladesh Journal of Scientific and Industrial Research (1976), 11(1-4), 148-53
CODEN: BJSIBL; ISSN: 0304-9809
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Four acetylenic compds. and Me linoleate were hydrogenated and deuterated using H and D containing Ni W8, W9, and W10 catalysts, e.g., Me(CH2)7C.tplbond.C(CH2)7CO2Me gave Me(CH2)7CH:CH(CH2)7CO2Me and Me(CH2)7CD:CD(CH2)7CO2Me. Oxygenation of the reduced products showed that the deutero-compds. have higher induction period than the corresponding H compds.

CC 23-17 (Aliphatic Compounds)

IT **Deuteration catalysts**
Hydrogenation catalysts
(nickel, for acetylenic compds. and methyl linolenate)

IT **Deuteration**
Hydrogenation
(of acetylenic compds. and methyl linolenate)

IT **7440-02-0**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for hydrogenation and deuteration of acetylenic compds. and methyl linolenate)

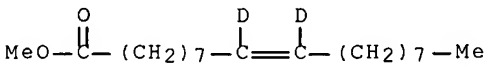
IT 2462-84-2P 2462-85-3P 5557-31-3P **56554-40-6P**
62439-46-7P 62439-47-8P 62439-48-9P 62439-49-0P
62439-50-3P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and oxygenation of)

IT **7440-02-0**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for hydrogenation and deuteration of acetylenic compds. and methyl linolenate)

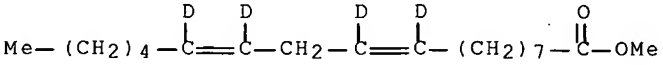
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

IT **56554-40-6P 62439-46-7P 62439-50-3P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and oxygenation of)

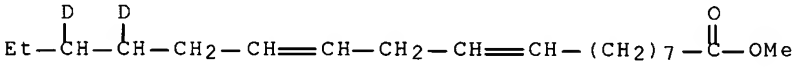
RN 56554-40-6 CAPLUS
CN 9-Octadecenoic-9,10-d2 acid, methyl ester (9CI) (CA INDEX NAME)



RN 62439-46-7 CAPLUS
CN 9,12-Octadecadienoic-9,10,12,13-d4 acid, methyl ester (9CI) (CA INDEX NAME)



RN 62439-50-3 CAPLUS
CN 9,12-Octadecadienoic-15,16-d2 acid, methyl ester (9CI) (CA INDEX NAME)



Compound of Claim 12:

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L26           2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L25
L27             STR
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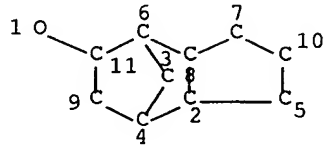

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  11

STEREO ATTRIBUTES: NONE
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L29         133 SEA FILE=CAPLUS ABB=ON  PLU=ON  L28
L30      168165 SEA FILE=CAPLUS ABB=ON  PLU=ON  ?DEUTER?
L31           4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L29 AND L30
L32           6 SEA FILE=CAPLUS ABB=ON  PLU=ON  L31 OR L26


=> d l32 ibib abs hitind hitstr tot

L32  ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2004:589514  CAPLUS  Full-text
DOCUMENT NUMBER:         141:139883
TITLE:                   Method of catalytic deuteration of carbonyl
                         compounds or secondary alcohols by heavy water
INVENTOR(S):             Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige;
                         Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S):      Wako Pure Chemical Industries, Ltd., Japan
SOURCE:                  PCT Int. Appl., 42 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                Japanese
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2004060831         A1    20040722    WO 2003-JP14182          20031107
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2511885	A1	20040722	CA 2003-2511885	20031107
AU 2003277596	A1	20040729	AU 2003-277596	20031107
EP 1577280	A1	20050921	EP 2003-814536	20031107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR; IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1732135	A	20060208	CN 2003-80107483	20031107
US 2006116535	A1	20060601	US 2005-539188	20050616
IN 2005KN01449	A	20070720	IN 2005-KN1449	20050726
PRIORITY APPLN. INFO.:			JP 2002-378932 A	20021227
			WO 2003-JP14182 W	20031107

OTHER SOURCE(S): CASREACT 141:139883; MARPAT 141:139883

AB Described is a method of **deuterating** a carbonyl or secondary alc. compound represented by the general formula R1-X-R2 (I) (wherein R1 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aralkyl ; R2 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aryl, aralkyl, alkoxy, aryloxy, hydroxy; X carbonyl, hydroxymethylene), which comprises reacting the compound represented by the general formula I with a **deuterium** source, in particular D2O, in the presence of a catalyst selected among activated palladium, platinum, rhodium, ruthenium, nickel, and cobalt catalysts. By the method, **deuteration**, which has been conducted under severe conditions, can be conducted under neutral conditions. Even when the compound contains an unsatd. bond, it can be **deuterated** without reducing the unsatd. bond. Not only hydrogens near the carbonyl or hydroxymethylene group but also those remotely situated from these groups are selectively **deuterated** without **deuterating** the carbon-carbon double or triple bonds. Thus, 500 mg tricyclo[5.2.1.02'6]decan-8-ol and 100 mg Pd-C were suspended in 17 mL D2O, purged with H, and heated at 180° for 24 h in an oil bath to give tricyclo[5.2.1.02'6]decan-8-ol **deuterated** by 96% at 8-position and 88% at other positions.

IC ICM C07B059-00
ICS C07C029-00; C07C031-02; C07C035-08; C07C035-29; C07C035-37; C07C045-00; C07C049-04; C07C049-08; C07C049-433; C07C049-453; C07C051-00; C07C053-10; C07C053-124; C07C057-04; C07M005-00

CC 21-2 (General Organic Chemistry)

ST **deuterated** carbonyl compd secondary alc prepn; catalytic **deuteration** ketone carboxylic acid secondary alc; palladium platinum **deuteration** catalyst; heavy water **deuteration** carbonyl compd secondary alc

IT **Deuteration**
Deuteration catalysts
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT Carbonyl compounds (organic), reactions
Carboxylic acids, reactions
Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(secondary; catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT 7440-02-0, Raney nickel, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts; catalytic **deuteration** of carbonyl compds. or

secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

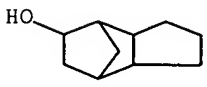
IT 7440-05-3, Palladium, uses 7440-05-3D, Palladium, supported on carbon 7440-06-4, Platinum, uses 7440-06-4D, Platinum, supported on carbon 7440-16-6, Rhodium, uses 7440-16-6D, Rhodium, supported on alumina 7440-16-6D, Rhodium, supported on carbon 7440-18-8, Ruthenium, uses 7440-18-8D, Ruthenium, supported on carbon 7440-48-4, Cobalt, uses
RL: CAT (Catalyst use); USES (Uses)
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT 67-64-1, Acetone, reactions 78-93-3, 2-Butanone, reactions 79-31-2, Isobutyric acid 79-41-4, Methacrylic acid, reactions 106-35-4, 3-Heptanone 108-93-0, Cyclohexanol, reactions 108-94-1, Cyclohexanone, reactions 110-43-0, 2-Heptanone 123-19-3, 4-Heptanone 127-09-3, Sodium acetate 497-38-1, 2-Norbornanone 543-49-7, 2-Heptanol 589-55-9, 4-Heptanol 3385-61-3, Tricyclo[5.2.1.02,6]-3-decen-8-ol 5536-61-8, Sodium methacrylate 7789-20-0, Water-d2 **13380-89-7**, Tricyclo[5.2.1.02,6]decan-8-ol 13380-94-4, Tricyclo[5.2.1.02,6]decan-8-one 63870-91-7, Norbornenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT 79-31-2DP, Isobutyric acid, **deuterated** 108-93-0DP, Cyclohexanol, **deuterated** 666-52-4P, 2-Propanone-1,1,1,3,3,3-d6 **13380-89-7DP**, Tricyclo[5.2.1.02,6]decan-8-ol, **deuterated** 14044-94-1P 18153-61-2DP, Bicyclo[2.2.1]heptan-2-one-3,3-d2, **deuterated** 21273-02-9DP, Cyclohexan-1-d-ol, **deuterated** 51209-49-5P, Cyclohexanone-d10 53481-06-4P 55935-44-9P 63870-91-7DP, Norbornenol, **deuterated** 64118-21-4P 91468-78-9DP, Bicyclo[2.2.1]heptan-2-d-2-ol, **deuterated** 350820-09-6P 725242-18-2P, 4-Heptanone-d14 725242-19-3DP, **deuterated** 725242-21-7DP, **deuterated** 725242-22-8P, 2-Heptanone-d14 725242-23-9P, 3-Heptanone-d14 725242-24-0P, 2-Heptanol-d15 725242-25-1P, 4-Heptanol-d15 725242-26-2DP, **deuterated** 725242-27-3DP, **deuterated** 725242-28-4DP, **deuterated** **725242-29-5DP**, **deuterated** **725242-29-5P** **725242-30-8P** 725242-31-9P 725242-32-0DP, **deuterated**
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

IT **13380-89-7**, Tricyclo[5.2.1.02,6]decan-8-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

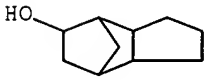
RN 13380-89-7 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro- (CA INDEX NAME)



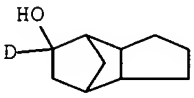
IT **13380-89-7DP**, Tricyclo[5.2.1.02,6]decan-8-ol, **deuterated**

725242-29-5DP, deuterated 725242-29-5P
725242-30-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalytic **deuteration** of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

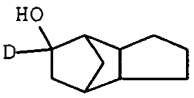
RN 13380-89-7 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro- (CA INDEX NAME)



RN 725242-29-5 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



RN 725242-29-5 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro-5-d- (9CI) (CA INDEX NAME)



RN 725242-30-8 CAPLUS
CN 4,7-Methano-1H-inden-1,1,2,3,6,7,7-d7-5-ol, octahydro-2,3,3a,4,5,6,7,7a-d8- (9CI) (CA INDEX NAME)

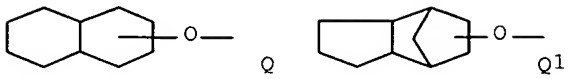
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:199410 CAPLUS Full-text
DOCUMENT NUMBER: 112:199410
TITLE: β-Methyl-δ-valerolactone adducts
INVENTOR(S): Kuroki, Masayuki; Yokoshima, Minoru; Maeda, Toshihiko; Yoshimura, Noriaki
PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan; Kuraray Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01258645	A	19891016	JP 1988-83125	19880406
PRIORITY APPLN. INFO.:			JP 1988-83125	19880406

GI



AB R(COCH2CHMeCH2CH2O)nH [R = R1C6H4O(CH2CHR2O)m, CpH2p+1O, perhydronaphthyloxy, perhydromethanoindanyloxy; R1 = H, C1-12 alkyl; R2 = H, Me; average m = 1-10; average n = 0.5-10; p = 1-20], whose (meth)acrylate esters are useful as diluents in UV-curable coatings, are prepared Thus, 374 parts poly(oxyethylene) p-nonylphenyl ether was treated with 684 parts β-methyl-δ-valerolactone at room temperature for 20 h to give 830 parts product with OH value 67.6.

IC ICM C07C069-675

CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 42

IT 126161-91-9P 126161-92-0P **126161-93-1P** 126161-94-2P
126286-45-1P 126286-48-4P 126305-36-0P
RL: PREP (Preparation)
(preparation of, as intermediate for methacrylate diluents, for UV-curable coatings)

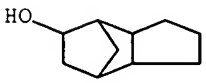
IT **126161-93-1P**
RL: PREP (Preparation)
(preparation of, as intermediate for methacrylate diluents, for UV-curable coatings)

RN 126161-93-1 CAPLUS

CN 2H-Pyran-2-one, tetrahydro-4-methyl-, homopolymer, octahydro-4,7-methano-1H-inden-5-yl ester (9CI) (CA INDEX NAME)

CM 1

CRN 13380-89-7
CMF C10 H16 O



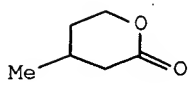
CM 2

CRN 97145-14-7

CMF (C6 H10 O2)x
CCI PMS

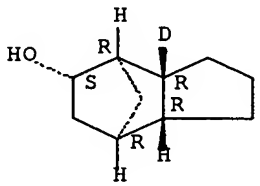
CM 3

CRN 1121-84-2
CMF C6 H10 O2



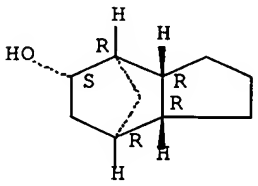
L32 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:81650 CAPLUS Full-text
DOCUMENT NUMBER: 80:81650
ORIGINAL REFERENCE NO.: 80:13137a,13140a
TITLE: Dehydration of 5-hydroxytetrahydro-exo-dicyclopentadiene with acid
AUTHOR(S): Gates, Marshall; Zabriskie, John L., Jr.
CORPORATE SOURCE: Dep. Chem., Univ. Rochester, Rochester, NY, USA
SOURCE: Journal of Organic Chemistry (1974), 39(2), p 222-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB A study of the dehydration of 3a-**deuterio**-5-hydroxytetrahydro-exo-dicyclopentadiene (I) with acid suggests that the formation of 5,6-dihydro-exo-dicyclopentadiene (II) proceeds through 2,3-dihydro-exo-dicyclopentadiene (III) or the equilibrating ions formed from the latter by protonation followed by a 1,3-hydride shift, a 1,2-hydride shift, and proton loss.
CC 22-3 (Physical Organic Chemistry)
IT **42913-50-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of)
IT **10271-44-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of, mechanism of)
IT **42913-50-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of)
RN 42913-50-8 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro-3a-d-, (3aα,4β,5β,7.beta.,7aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **10271-44-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of, mechanism of)
RN 10271-44-0 CAPLUS
CN 4,7-Methano-1H-inden-5-ol, octahydro-, (3aR,4R,5S,7R,7aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



L32 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:32153 CAPLUS Full-text
DOCUMENT NUMBER: 74:32153
ORIGINAL REFERENCE NO.: 74:5169a,5172a
TITLE: Polymerization of α-olefins
INVENTOR(S): Schmitt, Karl; Gude, Fritz; Samblebe, Reinhard
PATENT ASSIGNEE(S): Veba-Chemie A.-G.
SOURCE: Ger. Offen., 22 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1918995	A	19701112	DE 1969-1918995	19690415
AT 301169	B	19720825	AT 1970-1008	19700204
GB 1304093	A	19730124	GB 1970-7318	19700216
BE 746667	A	19700731	BE 1970-746667	19700227
NL 7003130	A	19701019	NL 1970-3130	19700305
FR 2039082	A5	19710108	FR 1970-10329	19700323
PRIORITY APPLN. INFO.:			DE 1969-1918995 A	19690415

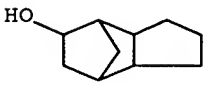
AB Ti(OBu)4, Ti(OPr)4, titanyl acetylacetonate, or a similar Ti compound, is used with VO(OBu)3, V acetylacetonate, or a similar V compound and with Et2AlCl, EtAlCl2, Et2AlBr, iso-Pr2AlBr, or a similar Al compound, optionally containing Et3Al and ZnCl2, Et2Zn, Et2Cd, or a similar compound, to prepare polymerization catalysts for C2H4, propylene, 4-methyl-1-pentene, and similar α-olefins. The catalysts have high catalytic activity, give colorless polymers even if the catalyst residue is not washed from the polymer, and give powdered polyolefins having good flow properties. Thus, 1 mole of a 1:3 molar mixture of Ti(OBu)4 and VO(OBu)3 in light petroleum was treated with 5.5 moles Et2AlCl to prepare a catalyst.
IC C08F001-42
CC 35 (Synthetic High Polymers)
IT 17501-79-0 19059-01-9 24742-16-3 28860-26-6 30860-71-0
32673-47-5 32673-53-3, Malonic acid, titanium(4+) salt (2:1)

32673-54-4 **32719-33-8**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polyn. of olefins)

IT **32719-33-8**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polyn. of olefins)

RN 32719-33-8 CAPLUS

CN 4,7-Methanoindan-5-ol, hexahydro-, titanium(4+) salt, exo- (8CI) (CA INDEX NAME)



●1/4 Ti(IV)

L32 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:432551 CAPLUS Full-text
DOCUMENT NUMBER: 61:32551
ORIGINAL REFERENCE NO.: 61:5679e-h,5680a-b
TITLE: Oxymercuration of endo- and exo-dicyclopentadienes
AUTHOR(S): Stille, J. K.; Stinson, S. C.
CORPORATE SOURCE: Univ. of Iowa, Iowa City
SOURCE: Tetrahedron (1964), 20(6), 1387-95
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:32551
GI For diagram(s), see printed CA Issue.

AB cf. Traylor and Baker, CA 59, 10101g. To 2.2 g. LiAlH4 in 15 ml. Et2O was added slowly 10.35 g. octahydro-exo-4,7-methanoinden-5-one in 20 ml. Et2O and the whole refluxed 1 hr. to give 6 g. octahydro-exo-4,7methanoinden- endo-5-ol (I), b1.5 73°, n19.5D 1.5127. The procedure of Cristol (C., et al., CA 54, 20908e) with I gave 52% octahydro-endo-methoxy-exo-4,7- methanoindene, b9 81°, n19.5D 1.4860. Hydroboration of 2,3,3a,4,7,7a-hexahydro-endo-4,7methanoindene gave octahydro-endo-4,7- methanoinden-exo-5-ol (II), m. 79.5-81° (MeNO2). II, as above, gave 47% octahydroexo-5-methoxy-endo-4,7-methanoindene (IIa), b6 84-6°, n19.5D 1.4923; CrO3 oxidation of II in C5H5N gave the ketone, which was reduced with LiAlH4 to give octahydro-endo-4,7-methanoinden- 5-ol (III), m. 119.5-20° (petr. ether). III gave 52% octahydroendo-5-methoxy-4,7-methanoindene, b9 81°, n19.5D 1.4860. HgCl2 and endo-dicyclopentadiene (IV) in MeOH gave 79% of the methoxymercuric chloride adduct (V), m. 133°; the same reaction with exo-cyclopentadiene (Va) proceeded twice as rapidly to give 50% of the adduct (Vb), m. 135-7°. Hg(OAc)2 (35 g.), 100 ml. H2O, and 10.7 g. IV shaken 10 hrs. gave 42% hydroxymercuric acetate adduct (VI), m. 129-31° (CCl4); a similar reaction with V was faster and gave 42% unstable adduct (VIa), m. 130-5° (CCl4). To 40 g. V in 400 ml. H2O, with agitation, was added in small portions 152 g. 3% Na-Hg, the whole extracted with Et2O, and the Et2O extract dried and concentrated gave, via vapor phase chromatography a 1:1 mixture (VII) of IV and VIII; pure VIII (9.7 g.) was obtained by distillation, b7 77-8°, n20D 1.5007. Similarly, Vb gave 50% IX, b9 81-3°, n19.5D 1.4976. VI gave 33% X, b4 91°, m. 42-4° (MeNO2) (p-nitrobenzoate m. 121.5-2.5°), and VIa

gave 12.5% XI, b3-5 92°, n19.5D 1.5262 (p-nitrobenzoate m. 126.5-8.5°). VIII (5.65 g.), EtOH, and PtO2 gave 3.6 g. IIa. Similarly, 4.8 g. IX gave 3.2 g. octahydroexo-5-methoxy-exo-4,7- methanoindene (XII), b7 81, n20D 1.4855, 2.28 g. X gave 1. 46 g. II, and 4.8 g. XI gave 1.58 g. octahydro-exo-4,7-methanoinden-exo-5-ol (XIII), m. 50.5-51°. V (20.4 g.), 200 ml. D2O, and 114 g. 3% Na-Hg gave 1.27 g. octahydro-exo-5-**deutero**-exo-6-methoxy-endo-4,7-methanoindene, b6 85-6°. The nuclear magnetic resonance spectra of some of these derivs. are discussed, the conclusion being that the mercuri group is cis or exo to the MeO or He groups.

CC 39 (Organometallic and Organometalloidal Compounds)

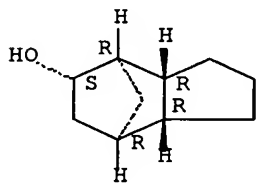
IT 77-80-5P, Tin, thiobis[triphenyl- 133-21-1P, 4,7-Methanoinden-5-ol, 3a,4,5,6,7,7a-hexahydro-(?), stereoisomers 338-48-7P, Germane, tributylfluoro 358-41-8P, Germane, triethylfluoro 994-28-5P, Germane, chlorotriethyl- 1067-10-3P, Germane, bromotriethyl- 1112-65-8P, Germane, acetoxytributyl 1441-22-1P, Tin, triphenyl(phenylthio)- 2117-36-4P, Germane, tributylchloro 2290-67-7P, Germane, triethylisothiocyanato- 2587-86-2P, Germane, oxybis[tributyl **10271-44-0P**, 4,7-Methanoindan-5-ol, hexahydro-, exo-exo- 13314-51-7P, Germane, triethyliodo- 22998-59-0P, Germane, dichlorodiisopropyl 24692-20-4P, Germanecarbonitrile, triethyl 53018-24-9P, 4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-5-methoxy-, stereoisomers 57831-55-7P, Germane, triethylisocyanato- 57879-96-6P, Tin, (methylthio)triphenyl- 79851-34-6P, Tin, (2-naphthylthio)triphenyl- 92168-27-9P, 4,7-Methanoinden-5-ol, 6-(acetoxymercuri)-3a,4,5,6,7,7a-hexahydro-, stereoisomers 93818-38-3P, 4,7-Methanoinden-5-ol, 3a,4,5,6,7,7a-hexahydro-(?), p-nitrobenzoate, stereoisomers 94522-39-1P, 4,7-Methanoindene-6-d, 3a,4,5,6,7,7a-hexahydro-5-methoxy- 104832-66-8P, 4,7-Methanoindan, hexahydro-5-methoxy-, exo-exo- 104832-66-8P, 4,7-Methanoindan, hexahydro-5-methoxy-, exo-exo- 104832-66-8P, 4,7-Methanoindan, hexahydro-5-methoxy-, exo-exo- 108172-97-0P, Mercury, chloro(3a,4,5,6,7,7a-hexahydro-5-methoxy-4,7-methanoinden-6-yl)-, stereoisomers
RL: PREP (Preparation)
(preparation of)

IT **10271-44-0P**, 4,7-Methanoindan-5-ol, hexahydro-, exo-exo-
RL: PREP (Preparation)
(preparation of)

RN 10271-44-0 CAPLUS

CN 4,7-Methano-1H-inden-5-ol, octahydro-, (3aR,4R,5S,7R,7aR)-rel- (CA INDEX NAME)

Relative stereochemistry.



L32 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:80843 CAPLUS Full-text
DOCUMENT NUMBER: 58:80843
ORIGINAL REFERENCE NO.: 58:13738e-h,13739a-d
TITLE: Bridged polycyclic compounds. XX. Cis stereochemistry

of the addition of methanol and water to endo-trimethylenenorbornene

AUTHOR(S): Cristol, Stanley J.; Gaston, Lyle K.; Johnson, Donald W.

CORPORATE SOURCE: Univ. of Colorado, Boulder

SOURCE: Tetrahedron Letters (1963) 185-9
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. CA 58, 10092d. H2SO4 catalyzed addition of MeOH (or of H2O in MeOH) to the isomeric endo-and exo-tri-methylenenorbornenes (I, II) gave differing ratios of endo (III) and exo (IV) ring skeleton ethers (or alcs.); e.g., I and MeOH was reported to give 14.5: 85.5 III (R = OMe) (V)-IV (R = OMe) (VI), and II with MeOH to yield 3.5: 96.5 V-VI. It is shown now that reactions with I are entirely cis-exo addns. If the endo protonated π complex (VII) reacted directly with a solvent mol. by the equivalent of trans ring opening, the addition of MeOD and D2O to I would lead to the compds. (VIII, R = OMe, OD) (IX, X). I and II lead to III and IV in such amts. that at least 80% of III from I arises via a path different from that utilized in the addition to II. If the alternative path involved VII, then at least 80% of the III isomer isolated in the **deuterated** series would be labeled as in VIII, and this would be true if VII were formed and gave III by isomerization to a carbonium ion (XI). If, however, VII is not involved in the reaction sequence, III might be expected to be labeled as in XII, assuming exo protonation followed by transformation to carbonium ion intermediates, coordinating with solvent from the exo side. It seemed that VIII and XII could be distinguished by differences in nuclear magnetic resonance (n.m.r.) spectra. III (R = OH) (XIII) in CHCl3 gave peaks at 6.07 (J 6.6 cycles/sec.), 7.6-9.2 τ. III (R = p-MeC6H4SO3, p-O2NC6H4CO2) showed similar doublets at 5.46 τ (J 6.6 cycles/sec.) and 4.90 τ (J 6.6 cyles/sec.). It appeared that the principal coupling was due to interaction between H and the C-3 H eclipsed with it, and that this coupling would be observed in XII, but would not appear in VIII. Treatment of 5,6-endo-trimethylene-2,3-exo-epoxynorbornane with LiAlD4 gave VIII (R = OH), showing a broad singlet at 6.02 τ; p-O2NC6H4CO2 derivative m. 123-6°, n.m.r. singlet at 4.89 τ. Addition of B2D6 to I followed by oxidation gave XII (R = OH), n.m.r. doublet at 6.09 τ (J 6.9 cycles/sec.); p-O2NC6H4CO2 derivative m. 128-9°, doublet at 4.99 τ (J 7.0 cycles/sec.). I (8.04 g. containing 9.7% II and 1.5% dicyclopentadiene), 5.5 ml. D2SO4, 2.2 ml. D2O, and 46 ml. MeOD refluxed 10 hrs. with stirring and treated with 10 g. Na2SO4, poured into H2O, and extracted with Et2O, the Et2O evaporated, and the residue [5.2% I, 10.3% V, 68.7% VI, 2.6% XIII, and 13.2% IV (R = OH) (XIV) by gas phase chromatography] chromatographed on Al2O3, eluted with pentane, and the ether mixture separated on a 2 m. (3/8 in.) 30% Carbowax 1540-Chromosorb column at 123° in 88 ml.He/min. gave I, XIV, and V in 26, 106, and 136 min. V showed a fairly sharp doublet at 6.74. τ (J.6.7) and the spectrum indicated that less than 10% of IX could be present as a contaminant in the XIII (R = OMe) produced. Further elution with Et2O gave the alc. fractions which were converted to p-nitrobenzoates inseparable into isomers. The esters reduced with LiAlH4, chromatographed on Al2O3, and separated by gas chromatography on a 1 m. (1/4 in.) 30% Carbowax 1540 column at 130° with 88 ml. He/min. gave XIV and XIII in 66 and 86 min., resp. XIII showed a doublet at 6.08 τ (J 6.6 cycles/sec.). Less than 10% of X could be present in the XII (R = OH) produced. Clearly cis-exo addition of both the H and R portions of the addenda occurs and the endo-protonated complex VII is excluded as a significant intermediate in the addition reaction to I leading to III. It is suggested that at least one of the intermediates involved is a classical ion

such as XI, or that a cis addition 4-center transition state is involved, in which no carbonium ion is developed.

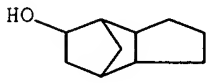
CC 32 (Physical Organic Chemistry)

IT 2198-08-5 2415-40-9 2628-89-9 **13380-89-7** 19398-83-5
68628-62-6 **96655-49-1** 97811-11-5
(Derived from data in the 7th Collective Formula Index (1962-1966))

IT **13380-89-7 96655-49-1**
(Derived from data in the 7th Collective Formula Index (1962-1966))

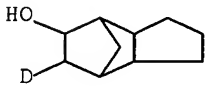
RN 13380-89-7 CAPLUS

CN 4,7-Methano-1H-inden-5-ol, octahydro- (CA INDEX NAME)



RN 96655-49-1 CAPLUS

CN 4,7-Methanoindan-6-d-5-ol, hexahydro- (7CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 15:58:41 ON 15 JAN 2008)

FILE 'CAPLUS' ENTERED AT 15:58:51 ON 15 JAN 2008
E US2005-539188/APPS
L1 1 SEA ABB=ON PLU=ON US2005-539188/AP
SEL RN
D SCA
E DEUTERATION/CT
E E3+ALL
L2 2077 SEA ABB=ON PLU=ON DEUTERATION+PFT/CT
E DEUTERATION CATALYSTS+ALL/CT
L3 287 SEA ABB=ON PLU=ON DEUTERATION CATALYSTS+PFT,NT/CT
L4 2148 SEA ABB=ON PLU=ON L2 OR L3

FILE 'REGISTRY' ENTERED AT 16:00:21 ON 15 JAN 2008

FILE 'CAPLUS' ENTERED AT 16:00:34 ON 15 JAN 2008
L5 TRA PLU=ON L4 1- RN : 22168 TERMS

FILE 'REGISTRY' ENTERED AT 16:01:30 ON 15 JAN 2008
L6 22168 SEA ABB=ON PLU=ON L5
L7 952 SEA ABB=ON PLU=ON L6 AND (PD OR PT OR RH OR RU OR NI OR CO)/ELS

FILE 'CAPLUS' ENTERED AT 16:03:17 ON 15 JAN 2008

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L8       154222 SEA ABB=ON  PLU=ON  L7(L)CAT+NT/RL
L9          247 SEA ABB=ON  PLU=ON  L8 AND L4
L10         115 SEA ABB=ON  PLU=ON  L2 AND L3 AND L8

     FILE 'REGISTRY' ENTERED AT 16:04:58 ON 15 JAN 2008
L11              STR

     FILE 'CAPLUS' ENTERED AT 16:10:55 ON 15 JAN 2008
                 S L11

     FILE 'REGISTRY' ENTERED AT 16:11:21 ON 15 JAN 2008
L12           50 SEA SUB=L6 SSS SAM L11

     FILE 'CAPLUS' ENTERED AT 16:11:21 ON 15 JAN 2008
L13           68 SEA ABB=ON  PLU=ON  L12

     FILE 'REGISTRY' ENTERED AT 16:11:26 ON 15 JAN 2008
L14           50 SEA SUB=L6 SSS SAM L11
L15         2492 SEA SUB=L6 SSS FUL L11
L16         1209 SEA ABB=ON  PLU=ON  L15 AND D/ELS

     FILE 'CAPLUS' ENTERED AT 16:12:27 ON 15 JAN 2008
L17          897 SEA ABB=ON  PLU=ON  L16(L)PREP+NT/RL
L18           40 SEA ABB=ON  PLU=ON  L17 AND L9
L19           22 SEA ABB=ON  PLU=ON  L17 AND L10
L20            1 SEA ABB=ON  PLU=ON  L1 AND L1

     FILE 'CAPLUS' ENTERED AT 16:13:16 ON 15 JAN 2008
                 D QUE L19
                 D L19 IBIB ABS HITIND HITSTR TOT
                 SEL RN L1

     FILE 'REGISTRY' ENTERED AT 16:15:20 ON 15 JAN 2008
L21           49 SEA ABB=ON  PLU=ON  (7440-16-6/BI OR 108-93-0/BI OR 13380-89-7/
                 BI OR 63870-91-7/BI OR 725242-29-5/BI OR 7440-05-3/BI OR
                 7440-06-4/BI OR 7440-18-8/BI OR 79-31-2/BI OR 106-35-4/BI OR
                 108-94-1/BI OR 110-43-0/BI OR 123-19-3/BI OR 127-09-3/BI OR
                 13380-94-4/BI OR 14044-94-1/BI OR 18153-61-2/BI OR 21273-02-9/B
                 I OR 3385-61-3/BI OR 350820-09-6/BI OR 497-38-1/BI OR 51209-49-
                 5/BI OR 53481-06-4/BI OR 543-49-7/BI OR 5536-61-8/BI OR
                 55935-44-9/BI OR 589-55-9/BI OR 64118-21-4/BI OR 666-52-4/BI
                 OR 67-64-1/BI OR 725242-18-2/BI OR 725242-19-3/BI OR 725242-21-
                 7/BI OR 725242-22-8/BI OR 725242-23-9/BI OR 725242-24-0/BI OR
                 725242-25-1/BI OR 725242-26-2/BI OR 725242-27-3/BI OR 725242-28
                 -4/BI OR 725242-30-8/BI OR 725242-31-9/BI OR 725242-32-0/BI OR
                 7440-02-0/BI OR 7440-48-4/BI OR 7789-20-0/BI OR 78-93-3/BI OR
                 79-41-4/BI OR 91468-78-9/BI)
L22           10 SEA ABB=ON  PLU=ON  L21 AND NR>2
                 D SCA
L23            2 SEA ABB=ON  PLU=ON  L22 AND ?DECAN?/CNS
                 D SCA
L24            1 SEA ABB=ON  PLU=ON  L23 AND C10H16O/MF
                 D
                 SEL RN
L25            3 SEA ABB=ON  PLU=ON  13380-89-7/CRN
                 D SCA

     FILE 'CAPLUS' ENTERED AT 16:17:52 ON 15 JAN 2008
L26            2 SEA ABB=ON  PLU=ON  L25
                 D QUE L26
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              D L26 IBIB ABS HITSTR TOT

     FILE 'REGISTRY' ENTERED AT 16:18:52 ON 15 JAN 2008
L27             STR 13380-89-7
L28          52 SEA FAM FUL L27

     FILE 'CAPLUS' ENTERED AT 16:19:11 ON 15 JAN 2008
L29         133 SEA ABB=ON  PLU=ON  L28
L30      168165 SEA ABB=ON  PLU=ON  ?DEUTER?
L31           4 SEA ABB=ON  PLU=ON  L29 AND L30
L32           6 SEA ABB=ON  PLU=ON  L31 OR L26

     FILE 'CAPLUS' ENTERED AT 16:19:51 ON 15 JAN 2008
              D QUE L32
              D L32 IBIB ABS HITIND HITSTR TOT
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